Quantized excitation spectra by magnon confinement in quasi-one-dimensional $S=1$ spin systems

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We apply the infinite time-evolving-block-decimation algorithm to calculate the dynamical spin-structure factors of the quasi-one-dimensional (q1D) $S=1$ antiferromagnetic spin system with the single-ion anisotropy and the bond alternation. We find that excitation continuum originating from magnons is quantized, when the staggered field induced by the weak inter-chain interaction is taken into account. The excitation energies of the quantized excitation spectra are well explained by negative zeros of the Airy functions, when the easy-axis anisotropy is strong and the ground state is located deep in the Néel phase. This quantization of the magnon continuum is a counterpart of the spinon confinement, which has been recently discussed in q1D $S=1/2$ antiferromagnets. We further show that, when the staggered field exists, the quantized excitation spectra appear the phase boundary between the Haldane phase and the Néel phase of the phase diagram without the staggered field. However, the quantized excitation spectra disappear in the singlet dimer phase.

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Recent inelastic neutron scattering (INS) experiment$^{[12]}$ on the quasi-one-dimensional (q1D) $S=1/2$ antiferromagnetic (AF) Ising-like XXZ magnets, (Ba/Sr)Co$_2$V$_2$O$_8$,$^{[1]}$ have reported that, below the Néel temperature, $T_N$, these materials show the quantized excitation spectra whose excitation energies are well explained by the series of negative zeros of the Airy function (NZAF). McCoy and Wu$^{[2]}$ argued the relationship between the NZAF and the confinement of the domain-wall excitations by focusing on the excitation spectra of the S=1/2 ferromagnetic (FM) Ising chain under weak transverse and longitudinal magnetic fields$^{[3]}$. Since the ground state of this model is the fully polarized state, the low-energy excitation is achieved by flipping spins in an arbitrary length, namely two domain-wall excitations. When we apply the mean-field treatment for the weak inter-chain interaction, the staggered fields are induced in the intra-chain Hamiltonian. The effective Hamiltonian

\[
\mathcal{H} = J \sum_{ij} (1 + \alpha (-1)^{i}) \mathbf{S}_{i,j} \cdot \mathbf{S}_{i+1,j} + D \sum_{ij} S_{i,j}^z \mathbf{S}_{i} \cdot \mathbf{S}_{i,j'}, \tag{1}
\]

where $i$ is the site index in the chain direction and $j$ specifies the chain. $J(>0)$ is antiferromagnetic intra-chain interaction and $J'(>0)$ is the inter-chain interaction. $\alpha$ denotes the bond alternation in the spin-chain direction. $D$ represents the single-ion anisotropy. The summation $\langle j,j' \rangle$ runs over all nearest-neighbor inter-chain pairs. We suppose the bipartite systems.

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\]
J allows us treat Hilbert space is still classified by the parity of total \( h_s \) is included, the total \( S_z \) is not a good index, but the Hilbert space is still classified by the parity of the total \( S_z \).

\[
\mathcal{H}_{\text{MF}} = J \sum_i (1 + \alpha(-1)^i) S_i \cdot S_{i+1} + D \sum_i S_i^2 + h_s \sum_i (-1)^i S_i^z, \tag{2}
\]

where \( h_s \) is the mean field derived from the magnetic moments in the nearest-neighbor chains and is determined by solving a self-consistent equation. In the following calculations, we set a small value of \( h_s \), because it is not important to obtain \( h_s \) self-consistently from a given \( J' \).

We apply infinite time-evolving-block-decimation algorithm \( \text{IEB} \) to calculate the dynamical spin structure factor (DSF) for the Hamiltonian \( \mathcal{H} \). The details of the numerical techniques have been discussed in Ref. \( i \). We obtain the DSFs from the Fourier transform of the dynamical spin-spin correlation functions for a finite window size, \( N \), in the real space. To reduce numerical noises, we combine the Gaussian filtering method \( \text{GEM} \) in the Fourier transform. In the following calculations, we set \( \chi_{\text{max}} = 120 \) that corresponds to the maximum value of the bond dimension for tensors composing the wave function and \( N = 200 \) for the window size.

In Fig. 1 we show the DSFs of the Hamiltonian \( \mathcal{H} \) for \( (\alpha, D/J) = (0, -5) \). When \( (\alpha, D/J) = (0, -5) \) and \( h_s = 0 \), the ground state is in the Néel phase. Since the critical point between the Haldane and Néel phases exists at \( D_c / J = -0.36 \pm 0.01 \), we consider that \( (0, D/J) = (0, -5) \) is located deep in the Néel phase. For \( (\alpha, D/J) = (0, -5) \), an isolated mode appears in \( 0 \leq q_x \leq \pi \) in the low-lying excitation of \( S^{xx}(q_x, \omega) \) and \( S^{zz}(q_x, \omega) \) [Fig. 1(a) and (b)]. Above the isolated mode, the excitation continuum appears. These excitation continua are quantized by the finite value of \( h_s \) as shown in Fig. 1(c) and (d). In Fig. 1(e) and (f), we compare the NZAF and each excitation energy of the quantized excitation spectra at \( q_x = \pi \) and \( \pi / 2 \). We find that the excitation energies of the quantized spectra in both \( S^{xx}(q_x, \omega) \) and \( S^{zz}(q_x, \omega) \) are quantitatively explained by the NZAF. Note that the lowest quantized state is not the low-lying isolated mode.

Since each spin prefers the \( S^z = \pm 1 \) state for the negatively large \( D/J \), the system is mapped to the AF Ising chain at the Ising limit, \( D/J \to -\infty \) due to the positive \( J \). For the bipartite system, the AF Ising chain is equivalent to the FM Ising chain via spin rotations on one of the two sub-lattices. The mapped Hamiltonian is expressed as \( \mathcal{H}_{\text{FM}} = \mathcal{H}_0 + \mathcal{H}_1 \), where \( \mathcal{H}_0 = D \sum_i S_i^2 - J \sum_i S_i^x S_{i+1}^x - h_s \sum_i S_i^z \) and \( \mathcal{H}_1 = J \sum_i (S_i^+ S_{i+1}^+ + S_i^- S_{i+1}^-) \). The condition \( |D| / J \gg 1 \) allows us treat \( \mathcal{H}_1 \) as the perturbation. If \( h_s \) is positively infinitesimal, the ground state of \( \mathcal{H}_0 \) is the fully polarized state, \( \psi_1^+ = \cdots + + + + + + + + + \cdots \), where \(+\), \(-\), and \( -\) in the ket denotes \( S^z = 1 \), \( 0 \), and \( -1 \), respectively. When \( \mathcal{H}_1 \) is included, the total \( S_z \) is not a good index, but the Hilbert space is still classified by the parity of the total \( S_z \).

First, we consider the low-energy excitation in \( S^{xx}(q_x, \omega) \). The low-energy excitation in \( S^{xx}(q_x, \omega) \) is described by the dynamics of the state \( \psi_1^+ = S_i^+ |\psi_{\text{GS}}^+\rangle \). Since \( S_i^+ \propto (S_i^+ + S_i^-) \), this initial state is represented by the one magnon state, \( \psi_1^+ \propto \cdots + + + + + + + + + \cdots \). The parity of \( \psi_1^+ \) is different from that of the ground state. Since the energy cost to create \( \psi_1^+ \) is approximately \( \omega = |D| + 2J \), the isolated mode by \( \psi_1^+ \) appears at \( \omega = |D| + 2J \), when \( \mathcal{H}_1 \) is absence. When \( \mathcal{H}_1 \) acts on the site with \( S^z = 0 \), the further excited state appears above \( \psi_1^+ \): The \( S^z = 0 \) moves to the nearest-neighbor site with accompanying the site with \( S^z = -1, \cdots + + + + - + + + + \cdots \). This means that the domain composed by the \( S^z = -1 \) sites develops...
by acting $H_1$ on the site with $S^z = 0$ repeatedly. Therefore, the excitation continuum with the band center at $\omega \approx |D| + 4J$ appears above the excitation mode by the $\psi_1^+$ state. In the mapped Hamiltonian, $h_s$ works as the confinement potential for the domain with the $S^z = -1$ sites and thus, the excitation continuum is quantized by $h_s$.

Next, we consider the low-energy excitation in $S^{zz}(q_x, \omega)$. Since the initial state in the longitudinal component is given by multiplying the ground state at the site $i$ by $S_i^z$, the parity of total $S_i^z$ for the initial state is conserved. $H_1$ operation on a nearest-neighbor pair of the initial state creates the two-magnon state, namely $\psi_2^+ = |\cdots + + 00 + + + \cdots \rangle$. The energy cost for creating $\psi_2^+$ is $\omega \approx 2|D| + 3J$. For example, when $H_1$ acts on $\psi_2^+$ twice at the sites with $S^z = 0$, each magnon moves to the opposite direction, $|\cdots + + 0 -- 0 + + + \cdots \rangle$. Thus, the domain with the $S^z = -1$ sites develops by acting $H_1$ repeatedly on the site with $S^z = 0$. This means that the domain-wall excitation is also allowed for $\psi_2^+$ and the excitation continuum appears centered at $\omega \approx 2|D| + 4J$. In the same manner to the excitation continuum by $\psi_1^+$, the excitation continuum by $\psi_2^+$ is quantized by $h_s$.

The quantization of the excitation continua discussed above is explained by the NZAF, because the mechanism is similar to that discussed in the $S=1/2$ FM Ising spin chain. Namely the confinement of the domain walls. We consider that the above scenario is satisfied for $D/J = -5$, which implied that the system is near the Ising limit. From the analogy to the domain wall excitation in the $S=1/2$ FM Ising spin chain, it is expected that the domain wall excitation by $\psi_0^+ = |\cdots + + + -- + + \cdots \rangle$ appears in the low-energy excitation. However, the higher order process is required to create such state and the intensity is much suppressed in the present case.

In Fig. 2, we show the DSFs for $(\alpha, D/J) = (0, -0.2)$, where the ground state is in the Haldane phase when $h_s = 0$. For $h_s = 0$, the single-magnon isolated mode appears in the low-lying excitation at $q_x \approx \pi$ and the multi-magnon continuum appears above the isolated mode, which is schematically the same behavior as that of the isotropic case $D = 0$. Even for $(\alpha, D/J) = (0, -0.2)$, the quantization of the excitation continuum emerges for $h_s > 0$. However, the quantization is not clear in comparison with that for $D/J = -5$. In Fig. 2(e) and (f), we compare the NZAF and the excitation energies of the quantized spectra at $q_x = \pi$ and $\pi/2$. For $(\alpha, D/J) = (0, -0.2)$, the excitation energies of the quantized spectra in $S^{xx}(q_x, \omega)$ and $S^{zz}(q_x, \omega)$ deviate from the NZAF. Note that the energy of the third quantized state ($N=3$) in $S^{zz}(q_x = \pi, \omega)$ accidentally agrees with the NZAF. Therefore, we consider that the origin of the quantization in the excitation spectra is different from that in the Ising limit.

For $(\alpha, D/J) = (0, -0.2)$ and $h_s = 0$, the system is in proximity to the phase boundary between the Haldane and Néel phases. At the critical point, the energy gap closes and the system is described by the Tomonaga-Luttinger liquid in the low-energy limit, which is equivalent to the theory of the free boson fields. When the system departs from the critical point, the low-energy effective model is expressed by adding the family of $C_b \exp[i\phi]$ terms to the Lagrangian of free-boson field theory, where $\phi$ is the bosonic field and $b$ and $C_b$ are constants. Each $C_b \exp[i\phi]$ is classified into relevant or irrelevant, and the most relevant interaction opens the energy gap. This means that the sine-Gordon field theory qualitatively describes the low-energy part of the system in proximity to the phase boundary. In the excitation spectrum of the sine-Gordon field theory, several isolated modes originating from the soliton/anti-soliton and breather modes are present in addition to the excitation continuum. When the system approaches the critical point, the excitation continuum shifts to the lower energy region and the isolated modes become unstable by touching the lower edge of the excitation continuum. However, when the system leaves from the critical point, these isolated modes are placed below the lower-edge of the excitation continuum and thus, we observe the quan-
tized excitation spectra. We consider that this scenario for the quantized excitation spectra is valid in the vicinity of the two critical lines: One is dividing the Néel and Haldane phases and the other is the Néel and singlet-dimer phases, as shown in Fig. 3 (a).

![Diagram](image_url)

FIG. 3: (a) Schematic region where the quantized excitation spectra are observed. In the shaded area, the excitation continuum shows the quantization for $h_s > 0$. Black dots are critical points at $h_s = 0$ presented in Ref. $[28]$, "H", "N", "SD", and "LD" corresponds to the Haldane phase, Néel phase, singlet-dimer phase, and large-$D$ phase, respectively. (b)–(e) $S^{xx}(q_x, \omega)$ at $(\alpha, D/J) = (0, 0), (0, 25, -0.2), (0, 25, -0.5), (0, 6, -0.5)$ for $h_s = 0.05$. Open circle, triangle, square, and diamond in (a) correspond to the parameter used in (b)–(e) for $h_s = 0$, respectively. Note that we show the DSFs in the extended zone representation except for (b). White arrows in (b) are pointing the peak positions of the intensity.

In Fig. 3 (a), we schematically draw the region where the quantized excitation spectra appear for $h_s > 0$, which is represented by the shaded area. Figures 3(b)–(e) are the results at $(\alpha, D/J) = (0, 0), (0, 25, -0.2), (0, 25, -0.5), (0, 6, -0.5)$ for $h_s = 0.05$. Open circle, triangle, square, and diamond in Fig. 3(a) correspond to the parameters for $h_s = 0$, respectively. In comparison with the intensity at $q_x = \pi$ and $\omega = 0$ in $S^{xx}(q_x, \omega)$, the intensity of the quantized excitation spectra is quite weak deep in the Néel phase. Thus, we show the results for $S^{xx}(q_x, \omega)$. For $(\alpha, D/J) = (0, 0), (0, 25, -0.2), (0, 25, -0.5)$, the system with the first parameter is located in the Haldane phase and the latter two are in the Néel phase for $h_s = 0$. In such case, the excitation continuum in the DSF is quantized for $h_s > 0$, as shown in Figs. 3(b), (c), and (d). We find that the quantization of the spectra is smeared when the system approaches the phase boundary to the singlet-dimer phase. The quantized excitation spectra disappear in the singlet-dimer phase, as shown in Fig. 3(e). This is explained by considering the low-energy excitation for $D = 0$ and $\alpha \approx 1$. For $D = 0$ and $\alpha \approx 1$, the ground state is the direct product state of the singlet dimers. The low-energy excitation that has a potential to composes the excitation continuum is given by replacing two singlets to two triplets from the ground state. As $\alpha$ decreases from $\alpha = 1$, the two-triplet excitation composes the excitation continuum around $q_x = \pi$. However, the staggered field does not work as the confinement potential and rather localizes the triplet dimers with $S^z = 0$. Note that the energy of the triplet dimer with $S^z = \pm 1$ remains unchanged by the staggered field, which means that the confinement potential is absent.

At $D \to \infty$, the ground state is expressed by the direct product of $S^z = 0$ at each site, namely $\psi_0 = |\cdots 00000000\cdots \rangle$. The lowest-energy excitation from $\psi_0$ is given by the single-spin flipping, $\psi^+_0 = |\cdots 00000000\cdots \rangle$ or $\psi^-_0 = |\cdots 00000000\cdots \rangle$. The site carrying $S^z = \pm 1$ propagates by the hopping term, $S^+_i S^+_{i+1} + S^-_i S^-_{i+1}$, and $\psi^+_0$ composes the isolated mode. The candidate of the low-energy excitation that composes the excitation continuum is obtained by creating two $S^z = 1$ ($S^z = -1$) states at the neighboring sites, $\psi^+_2 = |\cdots 00000000\cdots \rangle$ or $\psi^-_2 = |\cdots 00000000\cdots \rangle$. The site carrying $S^z = \pm 1$ almost freely travels in the chain, and thus, they compose the excitation continuum. However, since all sites sandwiched by the two sites with $S^z = 1$ ($S^z = -1$) are filled by $S^z = 0$ due to the energy cost, the staggered field does not work as the confinement potential for these two sites with $S^z = 0$. Thus, the quantized excitation spectra are suppressed in the singlet-dimer phase.

So far, many $S=1$ chain materials have been synthesized. The most of them are considered to have the positive single-ion anisotropy, but the negative single-ion anisotropy has been reported for several materials. For example, $\text{Y}_2\text{BaNiO}_4[23]$ and $\text{SrNi}_2\text{V}_2\text{O}_6[25]$ have been evaluated as $D/J \approx -0.33$ and $\approx -0.057$. We believe that there are many compounds whose proper models have been unsettled precisely due to the large deviation from the ideal Haldane-gap system. In such compounds, there is a chance to find the quantized excitation spectra. Further experiments are desirable.

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Supplemental Materials: Quantized excitation spectra by magnon confinement in quasi-one-dimensional $S=1$ spin systems

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Benchmark test of dynamical spin structure factors by the iTEBD method

![Diagram](image)

**FIG. S1:** Dynamical spin-structure factor. (a) The $S=1$ AF Heisenberg chain. (b) The $S=1/2$ AF Heisenberg chain.

We apply the infinite time-evolving-block-decimation (iTEBD) algorithm$^{[S1,S2]}$ to calculate the dynamical spin structure factor (DSF)$^{[S3,S4]}$. The details of the numerical techniques have been discussed in Ref. $^{[S3]}$. In Fig. S1, we show the benchmark results for the DSFs of the $S=1$ and $S=1/2$ AF Heisenberg chains. In the computations, we set $\chi_{\text{max}}= 80$, which is the maximum bond dimension of the matrix-product-state representation for the wave function, and $N = 200$ for the finite-size window$^{[S3]}$.

In the $S=1$ AF Heisenberg chain, we find that the result succeeds in reproducing the low-lying excitation of the Haldane-gap state, which has been already demonstrated in the previous works$^{[S3,S5]}$. The isolated mode by a single magnon with the energy gap $\omega_H/J \sim 0.41$ at $q_x = \pi$ and the lower-edge of the two-magnon continuum with the energy gap $\omega \sim 2\omega_H$ at $q_x \approx 0^\geq$. In the low-lying excitation, the isolated mode appears for $0.3 \leq q_x \leq \pi$ and becomes unstable for $0 \leq q_x \lesssim 0.3^\leq$. Above the single-magnon mode, the excitation continuum appears at $q_x \approx \pi$. The lower-edge of the continuum is composed by the three-magnon excitation$^{[S7]}$.

For the $S=1/2$ AF Heisenberg chain, we reproduce the dispersion relation given by des Cloizeaux and Pearson$^{[S8]}$ and the upper boundary of the spinon continuum$^{[S9,S11]}$. Although it is difficult to confirm the singularity of the intensity at the lower edge and higher edge of the excitation continuum quantitatively, the well-known spinon continuum is reproduced qualitatively$^{[S8,S12]}$.

Quantized spectra in the $S=1$ bond-alternating spin chain

In the main text, we only show $S^{xx}(q_x, \omega)$ for $h_s > 0$. In this supplemental material, we show the details of $S^{xx}(q_x, \omega)$ and $S^{zz}(q_x, \omega)$ for $h_s = 0$ and $h_s > 0$. Figures S2(a)–(t) are the results for $(\alpha, D/J) = (0, 0), (0.25, -0.2), (0.5, -0.5), (0.6, -0.5)$, and $(0.5)$. The definitions of $\alpha$, $D$, $h_s$ are presented in the main text. When the system is located in the Haldane phase with $D \lesssim 0$, the quantized excitation spectra appears in $S^{xx}(q_x, \omega)$ and $S^{zz}(q_x, \omega)$ [Figs. S2(b) and (l)]. The quantized excitation spectra in $S^{xx}(q_x, \omega)$ become clear for $h_s > 0$, as the system moves to the deep Néel phase [Figs. S2(d) and (f)]. Although, in the deep Néel phase, $S^{zz}(q_x, \omega)$ shows the quantized excitation spectra, the quantization is not clear because the peak at $\omega \approx 0$ shows the quite large intensity [Figs. S2(n) and (p)]. When the system is in the singlet-dimer phase, the staggered field does not contribute the confinement of the domain-wall excitation. Thus, the quantized excitation spectra do not appear, as shown in Figs. S2(h), (i), (r), and (t).

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FIG. S2: (a)–(j) $S^{xx}(q_x, \omega)$. (k)–(t) $S^{zz}(q_x, \omega)$. From the top row to the bottom row, the results for $(\alpha, D/J) = (0,0)$, $(0.25, -0.2)$, $(0.5, -0.5)$, $(0.6, -0.5)$, and $(0,5)$ are presented, respectively. The leftmost column (second column) and the third column (rightmost column) are the results for $h_s = 0$ ($h_s > 0$). White arrows are pointing peak positions.