Quantized $\Delta S = 2$ Excitation Spectra by Confinement in an $S = 1$ Spin Chain

Takafumi Suzuki and Sei-ichiro Suga

Graduate School of Engineering, University of Hyogo, Himeji, Hyogo 671-2280, Japan

We calculate the dynamical spin-structure factor of the $S = 1$ Ising spin chain with single anisotropy and longitudinal magnetic fields using the infinite time-evolving-block-decimation algorithm. We show that when a transverse magnetic field is applied, both the $\Delta S = 2$ excitation continuum and one-magnon mode appear in the low-lying excitation. When a longitudinal magnetic field is further applied, the excitation continuum changes into quantized excitation spectra. The quantized $\Delta S = 2$ excitation spectra originate from the confinement of two domain walls, each of which carries $\Delta S = 1$. The quantized excitation energies are explained by the negative zeros in the Airy function.

In a seminal study for the $S = 1/2$ ferromagnetic (FM) Ising spin chain in weak transverse and longitudinal magnetic fields, it was unveiled that quantized excitation spectra appear by the confinement of the domain-wall excitation.\(^1\) The lowest excitation of the $S = 1/2$ FM Ising spin chain is achieved by flipping the spins of arbitrary lengths. Each domain wall of both ends carries $\Delta S = 1/2$, namely spinon. In the transverse magnetic field, two spinons travel in the chain and compose an excitation continuum. When the longitudinal magnetic field is further weakly applied, it works as a confinement potential between two spinons, yielding the quantized excitation spectra whose excitation energies are described by the series of negative zeros in the Airy function (NZAF).\(^1\) The quantized spectra described by the NZAF have been confirmed in an elastic neutron scattering (INS) experiment\(^2\) on CoNb$_3$O$_6$, which is a FM Ising-spin-chain compound.

The quantized excitation spectra of the quasi-one-dimensional (q1D) $S = 1/2$ antiferromagnetic (AF) Heisenberg spin system have also been elucidated.\(^3\) Recently, the quantized excitation spectra of the q1D $S = 1/2$ AF Ising-like XXZ magnets, (Ba/Sr)Co$_2$V$_2$O$_6$,\(^4\) have been observed in the INS experiments.\(^5,6\) In these q1D AF spin systems, the excitation continuum originating from spinons appears in the low-lying excitation above the Neél temperature ($T_N$). Below $T_N$, an effective staggered field that works as a confinement potential is induced in the spin chain. Thus, the observed quantized excitation energies\(^5,6\) are explained by the NZAF in the similar manner to the discussion of the FM Ising-spin chain. This scenario has been further applied to systems in which the excitation continuum is generated by quasiparticles. The $S = 1$ AF Heisenberg chain is a typical system where the excitation continuum is generated by multimagons.\(^7,13\) We calculated the dynamical spin structure factor (DSF) of the q1D $S = 1$ AF Heisenberg system with single anisotropy, and demonstrated that quantized excitation spectra appear.\(^1,13\) The quantized excitation energies are well described by the NZAF, when the single-anisotropy is negatively strong.

In the INS experiment, neutrons are scattered by changing spins in the target systems by $\Delta S = 1$, which makes it possible to detect the low-lying excitation that composes the excitation continuum. The quantized excitation spectra in $S = 1/2$ spin systems have been observed in the INS experiments,\(^2,5,6\) because the $\Delta S = 1$ excitation generates the original excitation continuum. The quantized excitation spectra in the q1D $S = 1$ AF Heisenberg system with single anisotropy are possibly observed in the INS experiment, because its excitation continuum is generated by the multimagons with each magnon carrying $\Delta S = 1$.\(^1,13\) In this Letter, we show that the quantized $\Delta S = 2$ excitation spectra are generated in the DSF of an $S = 1$ spin chain. The quantized $\Delta S = 2$ excitation spectra provide observations in the INS experiment.

We consider the $S = 1$ FM Ising spin chain with single anisotropy in weak transverse and longitudinal magnetic fields. The Hamiltonian is written as

$$\mathcal{H} = J \sum_i S_i^x S_{i+1}^x + D_z \sum_i (S_i^z)^2 - H_z \sum_i S_i^z - H_x \sum_i S_i^x,$$  \hspace{1cm} (1)

where $J < 0$ and the single-anisotropy $D_z < 0$. In the following calculations, we focus on the system whose ground state is in the FM state for $H_z = 0$.

We apply the infinite time-evolving-block-decimation algorithm\(^1,15\) to calculate the DSF. The DFS is defined as $S^{\text{ms}}(q, \omega) = \pi^{-1} \text{Im} \int \left( \langle S_{\vec{r}}^z(t) S_{\vec{r}'}^z(0) \rangle e^{i \omega t} \delta(\vec{r} - \vec{r}') \right) dt$, where $\mu = x, y, z$ and $\varepsilon_z$ is the ground-state energy. The details of the numerical techniques have been discussed in Ref.\(^6\)

To reduce numerical noise, we combine the Gaussian filtering method\(^7\) with the Fourier transformation. In the following calculations, we set $\chi_{\text{max}} = 80$ and $N = 200$, where $\chi_{\text{max}}$ is the maximum bond dimension for tensors comprising the wave function and $N$ is the real-space window size for the Fourier transformation, respectively.

In Figs. 1(a) and 1(c), $S^{\text{ms}}(q, \omega)$ is shown for $(J, D_z, H_z) = (-0.25, -0.1, 0.45)$. Note that the same behavior is observed for $S^{\text{ms}}(q, \omega)$. We investigate the phase transition between the FM and paramagnetic states driven by $H_z$. For $(J, D_z) = (-0.25, -1)$ and $H_z = 0$, we confirm that the phase transition occurs at $H_z \approx 0.75$. For $H_z = 0$, the excitation continuum appears below $\omega |D_z| < 1.5$. When $H_z$ is switched on, the excitation continuum changes to the quantized spectra. We discuss the feature of the quantized spectra in $S^{\text{ms}}(q, \omega)$. For small $H_z$ and $H_x$, we divide $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$, where $\mathcal{H}_0 = \sum_i S_i^z S_{i+1}^z + D_z \sum_i (S_i^z)^2$ and $\mathcal{H}_1 = -H_z \sum_i S_i^z - H_x \sum_i S_i^x$. The ground state of $\mathcal{H}_0$ is the fully polarized state expressed by $\psi_{\text{GS}}^{\text{spin}} = \cdots \cdots |0 \cdots 1 \cdots 0 \cdots \cdots \rangle$ or $\psi_{\text{GS}}^{\text{oxy}} = \cdots \cdots |0 \cdots 0 \cdots 1 \cdots \cdots \rangle$, where $+1, 0$, and $-1$ in the ket denote $S_i^z = 1, 0,$ and $-1$, respectively. In the following discussion, we adopt the former ground state, $\psi_{\text{GS}}^{\text{spin}}$. The low-lying excitation in $S^{\text{ms}}(q, \omega)$ is described by the dynamics of the excited state whose initial
state is $\tilde S^i \psi^+_{GS} \propto S^i \psi^+_{GS}$. Thus, this initial state is interpreted as a one-magnon state, $|\cdots +++0+\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cd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spinon confinement. Since the DSF can be observed by INS experiments, we expect the present quantized $\Delta S = 2$ excitation spectra to be detected by INS experiments.

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\[ \sum \left( S^z_i S^z_{i+1} + S^+_i S^-_{i+1} \right)^{13.1} \]