Bound states of spinons in spatially anisotropic frustrated XXZ models in the Ising limit

Masanori Kohno
Computational Materials Science Center, National Institute for Materials Science, Tsukuba 305-0047, Japan
E-mail: KOHNO.Masanori@nims.go.jp

Abstract. Dynamical properties of frustrated XXZ models in the Ising limit on spatially anisotropic two-dimensional lattices are investigated by a weak-coupling approach from the one-dimensional limit. Restricting the Hilbert space to that spanned by exact eigenstates of XXZ chains in the Ising limit, we calculate dynamical structure factor $S^{+-}(k, \omega)$ in spatially anisotropic two-dimensional systems. As in the case of frustrated Heisenberg models [M.Kohno, et al., Nat. Phys. 3, 790 (2007)], spinons form bound states through hopping process between chains. We calculate the density-density correlation function of spinons in the Ising limit, and show that spinons in the bound state hop together as a pair, although those in a continuous spectrum behave almost independently. We discuss possible implications of the present results on fractionalization of bosonic and fermionic particles in spatially anisotropic frustrated systems with strong repulsion.

1. Introduction
Fractionalization of quantum numbers in elementary excitations of two-dimensional (2D) systems is one of the central subjects in modern condensed-matter physics. In unfrustrated antiferromagnets in dimensions higher than one, elementary excitations are well described by spin-wave theories [1, 2], and called magnons carrying $S^z=1$ [3]. On the other hand, in one-dimensional (1D) antiferromagnets, kinks between domains characterize the elementary excitations, which are called spinons carrying $S^z=1/2$ [4, 5]. Possibilities of fractionalization in 2D frustrated antiferromagnets have been theoretically suggested in various contexts: One of the pictures is based on the resonating valence bond (RVB) theory [6], where spinons are induced by breaking one of the resonating singlet bonds [7]. Another picture of spinons is topological defects among domains in 2D [8]. Also, constraint-fermion theories suggest fermionic spinons in 2D [9]. Although there are many interesting possibilities suggested, it is not so clear how spinons really behave in 2D.

To elucidate the properties of spinons in 2D, one practical approach may be to investigate crossover behaviors of 1D spinons to those in 2D by turning on weak interchain interactions between decoupled chains, because spinons are well defined at least in the 1D limit. Weak-coupling approaches from the 1D limit have been widely used to investigate low-energy properties. But, there have been fewer studies on excitations in energy scales of up to several times higher than exchange coupling $J$. In Ref. [10], we developed a new method which enables us to investigate properties of excitations in a wide range of energies. We applied this method to spatially anisotropic frustrated Heisenberg models, and successfully explained various puzzling
features observed in Cs$_4$CuCl$_4$ [11] without using any phenomenological fitting parameters [10]. In this paper, in order to clarify how 1D spinons are modified by interchain exchange processes, we apply this method to spatially anisotropic XXZ models in the Ising limit, where positions of spinons can be explicitly specified in a simple form.

2. Model
We consider spin-1/2 XXZ models on spatially anisotropic frustrated lattices. The Hamiltonian is defined as follows:

$$\mathcal{H} = \sum_{i,j=1}^{L} \left[ \frac{J_{xy}}{2} \left( S_{i,j}^+ S_{i+1,j}^- + S_{i,j}^- S_{i+1,j}^+ \right) + J_z S_{i,j}^z S_{i+1,j}^z \right] + \sum_{i,j=1}^{L} \sum_{\delta=0,\pm1} \left[ \frac{J'_{xy\delta}}{2} \left( S_{i,j}^+ S_{i+\delta,j+1}^- + S_{i,j}^- S_{i+\delta,j+1}^+ \right) + J'_{z\delta} S_{i,j}^z S_{i+\delta,j+1}^z \right],$$

where periodic boundary conditions are applied. The lattice structure is schematically shown in Fig. 1 (a). We focus attention on highly frustrated antiferromagnets which satisfy $J'_{\eta\delta}=J'_{\eta-1}+J'_{\eta1}$ ($\eta=xy$ and $z$), and assume $J_\eta > J'_{\eta\delta}$ so that the weak-coupling approach from the 1D limit works. We further take the Ising limit: $J_z, J'_{z\delta} \gg J_{xy}, J'_{xy\delta}$, which simplifies the wavefunctions and enables us to investigate the properties of spinons explicitly.

In particular, we consider the model on an anisotropic triangular lattice by taking $J'_{xy\delta}=J'_{\eta\delta}$ ($\equiv J'_{\eta}$) and $J'_{\eta-1}=0$ ($\eta=xy$ and $z$). We expect characteristics of dynamical properties in this model are generally realized in the models which satisfy the above conditions. We redefine unit vectors for the anisotropic triangular lattice as in Fig. 1 (b). The ground state of this model has collinear order as illustrated in Fig. 1 (c) [12].

3. Method
For the XXZ chain in the Ising limit, the eigenstates with $S^z=1$ are expressed in the site basis as [13]

$$|k_x, \epsilon \rangle = \frac{2\sqrt{2}}{L} \sum_{i,\alpha=1}^{L/2} e^{2ikx_i} e^{i\theta(\alpha-1)} \sin(q_j\alpha) \cdots \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \cdots,$$

where $\theta=-1+e^{2ikx}/(2|\cos k_x|)$ and $q_j=2\pi j/(L+2)$. The positions of spinons are denoted by $i$, which are located at $2i-0.5$ and $2i+2\alpha-1.5$. The energy $\epsilon$ at momentum $k_x$ is given as $\epsilon = J_z - 2J_{xy} |\cos k_x| |\cos q_j|$. 

![Figure 1](image-url)
Next, we consider the effects of interchain interactions. Restricting the Hilbert space to that spanned by the above eigenstates of the chain, we derive the effective Hamiltonian [10] for the XXZ model in the Ising limit on an anisotropic triangular lattice as:

$$H_{ij}^{\text{eff}} = \epsilon \delta_{i,j} + J'_{xy}(k) A(k_x, \epsilon') A(k_x, \epsilon'),$$  \hspace{1cm} (3)

where

$$J'_{xy}(k) = 2 J_{xy} \cos k_x \cos k_y \frac{k_x}{2}, \quad A(k_x, \epsilon') = \sqrt{\frac{2}{L}} \left( 1 - \frac{J_{xy} \cos k_x}{J_z} - \frac{\epsilon' - J_z}{J_z} \right) \sin q_j. \hspace{1cm} (4)$$

Diagonalizing this effective Hamiltonian numerically, we obtain eigenstates $|k, \epsilon_i\rangle$ and energies $\epsilon_i$ for spatially anisotropic 2D systems.

4. Results
We calculated the dynamical structure factor, which is expressed as

$$S^{+}(k, \omega) = M(k, \omega) D(k, \omega), \quad M(k, \epsilon_i) \equiv |\langle k, \epsilon_i| S_{k}^{+}(\text{G.S.})\rangle|^2 \quad \text{and} \quad D(k, \epsilon_i) = \frac{2}{\epsilon_{i+1} - \epsilon_{i-1}}, \hspace{1cm} (5)$$

where $M(k, \omega)$ is the transition rate from the ground state $|\text{G.S.}\rangle$, and $D(k, \omega)$ is the density of states. We took into account up to the first-order correction to the ground state.

Figure 2. Dynamical structure factor $S^{+}(k, \omega)$ for $J_{xy}/J_z=0.1$, $J'_{xy}/J_{xy}=0.4$ and $L = 960$. (a) $k_y=0$. (b) $k_y=\pi$ (c) $k_y=2\pi$. Insets show the intensity plot of $S^{+}(k, \omega)$.

Typical behaviors of the dynamical structure factor are shown in Fig. 2. Near $k_x = \pi/2$, $\delta$-functional peaks appear above and below the continuum for $J'_{xy}(k) > 0$ and $J'_{xy}(k) < 0$, respectively. This feature was also found in spatially anisotropic frustrated Heisenberg models, and explained the spectral features of Cs$_2$CuCl$_4$ [10].

Next, we consider correlations between spinons. We define the density-density correlation function of spinons as

$$N(\Delta x) \equiv L \sum_{x=0,5,1,5,\cdots} \langle k, \epsilon_i| n_{x,y} n_{x+\Delta x,y} |k, \epsilon_i\rangle, \hspace{1cm} (6)$$

where $n_{x,y}$ is the number operator of 1D spinons (kinks between domains). Using the eigenvector of the effective Hamiltonian $\{c^k_i\}$, we can rewrite this correlation function simply as $N(\Delta x) = 4 \sum_{j,l} c^k_i (\epsilon_j) c^k_l (\epsilon_l) \sin (q_j \Delta x) \sin (q_l \Delta x) / L$. The behaviors of density-density correlation functions are shown in Fig. 3. In the $\delta$-functional peaks of $S^{+}(k, \omega)$ below and above the continuum, the density-density correlation function has a sharp peak near $\Delta x \simeq 0$, which implies that two spinons strongly bind together and move coherently as a pair. In contrast, for the states in the continuum, the density-density correlation function of spinons does not show any characteristic structures, which implies that spinons move almost independently. This observation allows us to identify the $\delta$-functional peaks in $S^{+}(k, \omega)$ as bound and antibound states of spinons.
Figure 3. Density-density correlation function $N(\Delta x)$ for $J_{xy}/J_z=0.1$,  $J'_{xy}/J_{xy}=0.4$ and $L = 960$. (a) Bound state at $k=(0.5625 \pi, 2\pi)$. (b) Lowest-energy state of the continuum at $k=(0.59375 \pi, 2\pi)$. (c) Antibound state at $k=(0.5625 \pi, 0)$. The insets show $S^{-+}(k, \omega)$ at corresponding $k$. The arrows indicate the energy of the states.

5. Summary and discussion

In the corresponding fermionic systems, which are the spinless fermion models with large nearest-neighbor repulsions, two-peak structures of $S(\omega)$ were found by a numerical calculation in finite-size clusters [12]. These two peaks can be explained as formation of the above-mentioned bound and antibound states. The physical picture of the (anti)bound state is also consistent with that discussed in Ref. [12], where the peaks are interpreted as a result of the propagation of nonfractionalized particles in the perpendicular direction to the chain. Detailed analysis on the fermionic systems by the present approach will be shown elsewhere. The present results would also be true for other bosonic systems which can be effectively mapped onto the present models.

In summary, calculating density-density correlation functions of spinons in XXZ models in the Ising limit on anisotropic triangular lattices, we showed that, due to interchain hopping processes, spinons bind together and move coherently as a pair in the $\delta$-functional peaks of $S^{-+}(k, \omega)$. This behavior is contrasted with those in the continuous spectrum where no characteristic structure of the density-density correlation function is observed, which implies that spinons are almost uncorrelated in the continuum even in the presence of 2D exchange interactions.

Acknowledgments

I am grateful to L. Balents for stimulating discussions, helpful comments and useful suggestions. I would also like to thank C. Hotta and O.A. Starykh for discussions on related studies. This work was partly supported by KAKENHI 20740206 and 20046015, and World Premier international Research Center Initiative on Materials Nanoarchitectonics, MEXT, Japan.

References

[1] Anderson P W 1952 Phys. Rev. B 86 694
[2] Kubo R 1952 Phys. Rev. 87 568
[3] Bloch F 1930 Z. Phys. 61 206
[4] Faddeev L D and Takhtajan L A 1981 Phys. Lett. A 85 375
[5] Haldane F D M 1991 Phys. Rev. Lett. 66 1529
[6] Anderson P W 1973 Mater. Res. Bull. 8 153
[7] Kivelson S A, Rokhsar D S and Sethna J P 1987 Phys. Rev. B 35 8865
[8] Levin M and Senthil T 2004 Phys. Rev. B 70 220403
[9] Motrunich O I 2005 Phys. Rev. B 72 045105
[10] Kohno M, Starykh O A and Balents L 2007 Nat. Phys. 3 790
[11] Coldea R, Tennant D A and Tylczynski Z 2003 Phys. Rev. B 68 134424
[12] Hotta C and Pollmann F 2008 Phys. Rev. Lett. 100 186404
[13] Ishimaru N and Shiba H 1980 Prog. Theor. Phys. 63 743