Dynamical properties of spatially anisotropic frustrated Heisenberg models in a magnetic field

Masanori Kohno\textsuperscript{1}, Leon Balents\textsuperscript{2} and Oleg A. Starykh\textsuperscript{3}

\textsuperscript{1}International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Tsukuba 305-0047, Japan
\textsuperscript{2}Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106, USA
\textsuperscript{3}Department of Physics, University of Utah, Salt Lake City, UT 84112, USA

E-mail: KOHNO.Masanori@nims.go.jp

Abstract. We investigate spectral features of spatially anisotropic spin-1/2 frustrated antiferromagnets in a magnetic field by a weak-coupling approach from the one-dimensional (1D) limit. Using exact results of the Heisenberg chain, we calculate dynamical structure factors of spatially anisotropic frustrated antiferromagnets in two dimensions. We obtain rich peak structures depending on the momentum and the strength of magnetic fields. We identify the sharp peaks as bound and antibound states between particles carrying fractional $S_z$ in 1D in a magnetic field, psinons and antipsinons, and those originating from 2-string solutions. We compare these spectral features with available experimental results on Cs\textsubscript{2}CuCl\textsubscript{4}, and suggest that the dynamical properties of Cs\textsubscript{2}CuCl\textsubscript{4} in a magnetic field can be interpreted in terms of particles in 1D in a magnetic field.

1. Introduction

Particles carrying fractional $S_z$ have been theoretically suggested for two-dimensional (2D) frustrated antiferromagnets \cite{1, 2}. The frustrated antiferromagnet Cs\textsubscript{2}CuCl\textsubscript{4} has attracted much attention as an example which exhibits unusual dynamical features \cite{3, 4}. This material can be effectively regarded as a Heisenberg antiferromagnet on an anisotropic triangular lattice. The coupling constants were experimentally estimated as $J\simeq 0.374$ meV and $J'\simeq 0.128$ meV for intra- and interchain interactions, respectively \cite{5}. The dynamical structure factor observed in this material has a large spectral weight in a wide range of energies \cite{3, 4}, which is difficult to understand from conventional magnon pictures, but rather similar to the behaviors of one-dimensional (1D) chains. Inspired by this experimental study, many theories based on 2D spinons have been proposed \cite{6, 7, 8, 9, 10, 11} to explain the unusual dynamical behaviors. We investigated the dynamical properties by a weak-coupling approach from the 1D limit with use of exact solutions in 1D, and successfully explained not only the large tail of the dynamical structure factor but also the asymmetry of dispersion relations and the strong momentum dependence of lineshapes without using phenomenological parameters \cite{12}.

In a magnetic field, it is naively expected that classical antiferromagnetic orders may be suppressed, and exotic features may be relatively enhanced. Related to this point of view, not only spin-wave theories \cite{13, 14, 15} but also fermionic theories \cite{16} have been applied to 2D frustrated antiferromagnets in a magnetic field. For Cs\textsubscript{2}CuCl\textsubscript{4}, weak-coupling approaches from
Heisenberg chain in a magnetic field for $k$ of anisotropic 2D systems in a magnetic field. We use the exact transition rate of the
and $S$ lattices. The Hamiltonian is defined as follows:

$$H = \sum_{x,y} \left( J_S x+1,y + \sum_{\eta=0,\pm 1} J'_x S_{x+\eta,y+1} \right) \cdot S_{x,y} - H S^z,$$

where $S_{x,y}$ is the spin-1/2 operator at site $(x,y)$, and $S^z \equiv \sum_{x,y} S^z_{x,y}$. The intra- and interchain couplings are denoted by $J$ and $J'_x$ ($\eta=0,\pm 1$), respectively, as in Fig. 1 (a). We focus attention on highly frustrated antiferromagnets satisfying $J'_0=J'_1+J'$ and $J>J'_0,0>0 (\eta=0,\pm 1)$. In particular, we consider the model on an anisotropic triangular lattice by taking $J'_0=J'_1 (\equiv J')$ and $J'_1=0$. In the small $J'_0/J$ regime, basic dynamical features of this model are expected to be generally true for the models which satisfy the above conditions except properties in small energy scales.

We apply the method we developed in Ref. [12]: We restrict the Hilbert space to that spanned by the eigenstates of the Heisenberg chains, and derive the effective Hamiltonian as

$$[H^\alpha_{\text{eff}}(k)]_{i,j} = \epsilon_i \delta_{i,j} + J'(k) A^\alpha(k_x,\epsilon_i) A^{\alpha*}(k_x,\epsilon_j)/\xi_\alpha,$$

where $\xi_\alpha=1$ and 2 for $\alpha=z$ and $\pm$, respectively, and $A^\alpha(k_x,\epsilon_i) \equiv \langle k_x,\epsilon_i|S^\alpha_x|0\rangle$. Here, $|0\rangle$ and $|k_x,\epsilon_i\rangle$ denote the ground state and an excited state with excitation energy $\epsilon_i$ and momentum $k_x$ of the Heisenberg chain in a magnetic field, respectively. The Fourier component of interchain couplings is given by $J'(k)=4J' \cos(k_x/2) \cos(k_y/2)$ for anisotropic triangular lattices in the coordinates defined in Fig. 1 (b). Using the eigenstates of the effective Hamiltonian, we calculate dynamical structure factors in 2D, assuming the product ansatz [19]:

$$S^{\alpha}(k,\omega) = M^{\alpha}(k,\omega) D(k,\omega)$$

for $\alpha=z$ and $\pm$, where $M^{\alpha}(k,\epsilon_i) \equiv \langle k,\epsilon_i|\Sigma^\alpha|G.S.|^2$ and $D(k,\epsilon_i) \equiv 2/(\epsilon_{i+1}-\epsilon_{i-1})$. Here, $|G.S.|$ and $|k,\epsilon_i\rangle$ denote the ground state and an excited state with excitation energy $\epsilon_i$ and momentum $k$ of anisotropic 2D systems in a magnetic field. We use the exact transition rate of the Heisenberg chain in a magnetic field for $A^\alpha(k_x,\epsilon_i)$, which is expressed in a determinant form [20, 21, 22] using rapidities of Bethe-ansatz solutions [23].

**Figure 1.** Lattice structures and coupling constants. (a) General spatially anisotropic frustrated systems. (b) Anisotropic triangular lattice. The unit vectors are denoted by $\hat{x}$, $\hat{y}$, $\hat{x}'$, and $\hat{y}'$. 

the 1D limit based on renormalization-group analyses and the random-phase approximation have also been applied, and reasonably explained the observed behaviors in this material [17, 18]. In this paper, we apply the method we developed in Ref. [12] to spatially anisotropic frustrated antiferromagnets in a magnetic field to clarify the magnetic-field effects on the dynamical properties in a wide range of energies.

2. Model and method

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

$$H = \sum_{x,y} \left( J_S x+1,y + \sum_{\eta=0,\pm 1} J'_x S_{x+\eta,y+1} \right) \cdot S_{x,y} - H S^z,$$

where $S_{x,y}$ is the spin-1/2 operator at site $(x,y)$, and $S^z \equiv \sum_{x,y} S^z_{x,y}$. The intra- and interchain couplings are denoted by $J$ and $J'_x$ ($\eta=0,\pm 1$), respectively, as in Fig. 1 (a). We focus attention on highly frustrated antiferromagnets satisfying $J'_0=J'_1+J'$ and $J>J'_0,0>0 (\eta=0,\pm 1)$. In particular, we consider the model on an anisotropic triangular lattice by taking $J'_0=J'_1 (\equiv J')$ and $J'_1=0$. In the small $J'_0/J$ regime, basic dynamical features of this model are expected to be generally true for the models which satisfy the above conditions except properties in small energy scales.

We apply the method we developed in Ref. [12]: We restrict the Hilbert space to that spanned by the eigenstates of the Heisenberg chains, and derive the effective Hamiltonian as

$$[H^\alpha_{\text{eff}}(k)]_{i,j} = \epsilon_i \delta_{i,j} + J'(k) A^\alpha(k_x,\epsilon_i) A^{\alpha*}(k_x,\epsilon_j)/\xi_\alpha,$$

where $\xi_\alpha=1$ and 2 for $\alpha=z$ and $\pm$, respectively, and $A^\alpha(k_x,\epsilon_i) \equiv \langle k_x,\epsilon_i|S^\alpha_x|0\rangle$. Here, $|0\rangle$ and $|k_x,\epsilon_i\rangle$ denote the ground state and an excited state with excitation energy $\epsilon_i$ and momentum $k_x$ of the Heisenberg chain in a magnetic field, respectively. The Fourier component of interchain couplings is given by $J'(k)=4J' \cos(k_x/2) \cos(k_y/2)$ for anisotropic triangular lattices in the coordinates defined in Fig. 1 (b). Using the eigenstates of the effective Hamiltonian, we calculate dynamical structure factors in 2D, assuming the product ansatz [19]:

$$S^{\alpha}(k,\omega) = M^{\alpha}(k,\omega) D(k,\omega)$$

for $\alpha=z$ and $\pm$, where $M^{\alpha}(k,\epsilon_i) \equiv \langle k,\epsilon_i|\Sigma^\alpha|G.S.|^2$ and $D(k,\epsilon_i) \equiv 2/(\epsilon_{i+1}-\epsilon_{i-1})$. Here, $|G.S.|$ and $|k,\epsilon_i\rangle$ denote the ground state and an excited state with excitation energy $\epsilon_i$ and momentum $k$ of anisotropic 2D systems in a magnetic field. We use the exact transition rate of the Heisenberg chain in a magnetic field for $A^\alpha(k_x,\epsilon_i)$, which is expressed in a determinant form [20, 21, 22] using rapidities of Bethe-ansatz solutions [23].
In 1D, excitations are specified by the Bethe quantum numbers $\{I_j\}$ [23]. In a magnetic field, a hole and a particle created from the distribution of $\{I_j\}$ of the ground state are called psinon and antipsinon, and denoted by $\psi$ and $\psi^*$, respectively [19, 24]. We use dynamically dominant excitations of $O(L^2)$ states [19, 24, 25, 26] in a chain of length $L=2240$, and apply the method of Ref. [12] to each continuum separately to calculate dynamical structure factors in 2D.

3. Results

Figure 2 shows the behaviors of dynamical structure factors at $k_y=0$ for $J'/J=0.34$. For $J'(k)<0$, spectral weights shift to lower energies, and bound states are formed below continua as found in the zero-field case [12]. Typical behaviors are shown in the upper panels of Fig. 3. For $J'(k)>0$, on the other hand, spectral weights shift to higher energies, and antibound states appear above continua in some regions of the momentum space.

We compare the present results with the experimental results on Cs$_2$CuCl$_4$ [27] in Fig. 3. The peak positions of the observed lineshapes in the experiment [27] are reasonably explained as signatures of bound states. The low-energy peak can be interpreted as a superposition of the bound state of two $\psi$s in $S^{-+}(k,\omega)$ and that of $\psi$ and $\psi^*$ in $S^{zz}(k,\omega)$. The high-energy peak originates from 2-string solutions [23, 26].

4. Summary

We have investigated dynamical properties of spatially anisotropic frustrated antiferromagnetic Heisenberg models in a magnetic field by a weak-coupling approach from the 1D limit, using exact solutions of the Heisenberg chain. Depending on the momentum, bound and antibound states are formed for $J'(k)<0$ and $J'(k)>0$, respectively. Also, $S^{\alpha\alpha}(k,\omega)$ ($\alpha=z$ and $\pm$) exhibit different behaviors from each other in a magnetic field, which results in rich peak structures in the 2D momentum space. Comparing the present results with available experimental results on Cs$_2$CuCl$_4$, we interpret the peaks observed in the experiment [27] as signatures of bound states of fractional-$S^z$ particles, $\psi$ and $\psi^*$, and those of 2-string solutions. Detailed quantitative analyses including higher-order $\psi\psi^*$ excitations will be presented elsewhere [28].
**Figure 3.** Comparisons with experimental results on Cs$_2$CuCl$_4$ in magnetic fields [27] at $k=(3\pi/2,0)$ for (a) $H \approx 1$ T, (b) $H \approx 1.66$ T and (c) $H \approx 2$ T. (Upper panels) Red solid lines, green dashed lines and blue dotted lines denote the present results of $S^- (k, \omega)$, $S^z (k, \omega)$ and $S^{+-} (k, \omega)$, respectively. (Lower panels) Symbols are the experimental results taken from Ref. [27] for comparison. Here, the background is subtracted.

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**References**

[1] Anderson P W 1973 *Mater. Res. Bull.* **8** 153
[2] Kivelson S A, Rokhsar D S and Sethna J P 1987 *Phys. Rev. B* **35** 8865
[3] Coldea R, Tennant DA, Tsvelik A M and Tylczynski Z 2001 *Phys. Rev. Lett.* **86** 1335
[4] Coldea R, Tennant D A and Tylczynski Z 2003 *Phys. Rev. B* **68** 134424
[5] Coldea R et al. 2002 *Phys. Rev. Lett.* **88** 137203.
[6] Chung C H, Marston J B, McKenzie R H 2001 *J. Phys.: Condens. Matter* **13** 5159
[7] Zhou Y, Wen X G 2002 arXiv:cond-mat/0210662v3
[8] Chung C H, Voelker K, Kim Y B 2003 *Phys. Rev. B* **68** 094412
[9] Yunoki S and Sorella S 2004 *Phys. Rev. Lett.* **92** 157003
[10] Alicea J, Motrunich O I and Fisher M P A 2005 *Phys. Rev. Lett.* **95** 247203
[11] Isakov S V, Senthil T and Kim Y B 2005 *Phys. Rev. B* **72** 174417
[12] Kohno M, Starykh O A and Balents L 2007 *Nat. Phys.* **3** 790
[13] Veillette M Y, Chalker J T and Coldea R 2005 *Phys. Rev. B* **71** 214426
[14] Gan J Y, Zhang F C and Su Z B 2003 *Phys. Rev. B* **67** 144427
[15] Shen S Q and Zhang F C 2002 *Phys. Rev. B* **66** 172407
[16] Alicea J and Fisher M P A 2007 *Phys. Rev. B* **75**, 144411
[17] Starykh O A and Balents L 2007 *Phys. Rev. Lett.* **98** 077205
[18] Bocquet M, Essler F H L, Tsvelik A M and Gogolin A O 2001 *Phys. Rev. B* **64** 094425
[19] Karbach M and Müller G 2000 *Phys. Rev. B* **62** 14871
[20] Kitanine N, Maillet J M and Terras V 1999 *Nucl. Phys. B* **554** 647
[21] Biegel D, Karbach M and Müller G 2002 *Europhys. Lett.* **59** 882
[22] Caux J -S, Hagemans R and Maillet J M 2005 *J. Stat. Mech.* P09003
[23] Bethe H 1931 Z. Phys. **71** 205
[24] Karbach M, Biegel D and Müller G 2002 *Phys. Rev. B* **66** 054405
[25] Müller G, Thomas H, Beck H and Bonner J C 1981 *Phys. Rev. B* **24** 1429
[26] Kohno M (unpublished)
[27] Coldea R et al. 1997 *Phys. Rev. Lett.* **79** 151
[28] Kohno M (unpublished)