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Spin dynamics of a one-dimensional spin-1/2 fully anisotropic Ising-like antiferromagnet in a transverse magnetic field

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Abstract

We consider the one-dimensional Ising-like fully anisotropic $S = 1/2$ Heisenberg antiferromagnetic Hamiltonian and study the dynamics of domain wall excitations in the presence of a transverse magnetic field h_x . We obtain dynamical spin correlation functions along the magnetic field, $S^{xx}(q, \omega)$, and perpendicular to it, $S^{yy}(q, \omega)$. It is shown that the line shapes of $S^{xx}(q, \omega)$ and $S^{yy}(q, \omega)$ are purely symmetric at the zone boundary. It is observed in $S^{yy}(q, \omega)$ for $\pi/2 < q < \pi$ that the spectral weight moves toward the low-energy side with the increase of h_x . This model is applicable to the study of the spin dynamics of CsCoCl_3 in the presence of weak interchain interactions.

1. Introduction

The spin- $\frac{1}{2}$ Ising-like antiferromagnetic (AFM) chain has been the subject of theoretical studies for quite some time. The spin dynamics of the system is characterized by a picture of propagating domain walls or solitons. The magnetic compounds CsCoCl_3 and CsCoBr_3 are good examples of $S = \frac{1}{2}$ Ising-like AFM chains. The simplest exchange interaction Hamiltonian describing these compounds is the $S = \frac{1}{2}$ XXZ Heisenberg model

$$H_{XXZ} = 2J \sum_i [S_i^z S_{i+1}^z + \epsilon(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y)] \quad 0 < \epsilon < 1. \quad (1)$$

For very small ϵ , the lowest-order ground state of equation (1) is the Néel state with a z -component of the total spin given by $S_T^z = 0$. Villain [1] has calculated the longitudinal correlation function $S^{zz}(q, \omega)$ based on the basis states consisting of a single domain wall and predicted the appearance of a central peak with sharp shoulders. On the other hand, Ishimura and Shiba [2] proposed a picture of domain wall pair (DWP) states and showed that the propagating DWPs give rise to an excitation continuum around the Ising excitation energy $2J$. The transverse correlation function $S^{xx}(q, \omega)$ exhibits a broad peak around $2J$. The existence of these peaks of $S^{zz}(q, \omega)$ and $S^{xx}(q, \omega)$ has been verified by inelastic neutron

scattering experiments on CsCoCl₃ [3–5] and CsCoBr₃ [6]. A significant feature of the spin-wave response of $S^{xx}(q, \omega)$ near the zone centre ($q = \pi$) is that the spectral weights are heavily concentrated towards the lower-energy region. Nagler *et al* [6] added a staggered-field term

$$H_S = h \sum_i (-1)^i S_i^z \quad (2)$$

to the Hamiltonian in equation (1). The staggered field h has two contributions, h_0 and h_{ic} . The first contribution originates from taking account of the exchange mixing of higher levels with the ground doublet. The second contribution arises from the interchain exchange interactions at low temperatures. The interchain interactions treated in the mean-field approximation give rise to the staggered-field term h_{ic} . The effective Hamiltonian contains both the terms H_{XXZ} and H_S . With this effective Hamiltonian, the broad peak is found to split into discrete peaks which is known as the Zeeman ladder and observed in Raman scattering on CsCoCl₃ and CsCoBr₃ [7]. However, the observed line shapes of $S^{xx}(q, \omega)$ are quite different from those of the theoretical predictions. Matsubara and Inawashiro [8] have included a weak next-nearest-neighbour (NNN) ferromagnetic (FM) interaction H_F in the Hamiltonian H_{XXZ} in equation (1):

$$H_F = -2J' \sum_i [S_i^z S_{i+2}^z + \epsilon(S_i^x S_{i+2}^x + S_i^y S_{i+2}^y)]. \quad (3)$$

They have shown the existence of bound states of DWPs as well as the free DWP states, and the transverse correlation function $S^{xx}(q, \omega)$ exhibits a sharp peak in the lower-energy region.

The effect of a transverse magnetic field h_x on the spin dynamics of this model has been studied by Murao *et al* [9] who have shown that the spectral weight moves towards the low-energy side in $S^{yy}(q, \omega)$ for $\pi/2 < q < \pi$ with the increase in h_x , while there is no appreciable change in $S^{xx}(q, \omega)$ for all q . The distribution of intensities of the sharp peaks in $S^{yy}(q, \omega)$ varies irregularly for $q \approx \pi$. Although the proposed form of NNN FM coupling provides a good description of most of the experimental results, the required magnitude of the NNN exchange $|J'| \sim 0.1|J|$ is unphysically large [10]. In 1996, Bose and Ghosh [11] proposed the Ising-like fully anisotropic Heisenberg AFM Hamiltonian in 1D and showed that the asymmetric line shapes of $S^{xx}(q, \omega)$ and the bound states of DWPs can be derived.

In the absence of the magnetic field, S_T^z is a good quantum number and the eigenvalues of different S_T^z having unequal numbers of DWPs form different energy bands separated by energy $2J$. In the presence of a longitudinal magnetic field, h_z , S_T^z is still a good quantum number and the eigenvalues for the same value of S_T^z as well as the position of the peak of $S^{xx}(q, \omega)$ shift parallel with the increase in h_z . However, S_T^z is no longer a good quantum number in the presence of a transverse magnetic field h_x and a mixing of states with different S_T^z occurs. Thus, eigenvalues as well as eigenstates will be modified by h_x and the characteristics of the spin dynamics will be different.

In this paper, we study the effect of h_x on the dynamical spin correlation functions in a fully anisotropic Ising-like $S = \frac{1}{2}$ Heisenberg AFM chain at low temperatures. Dynamical correlation functions $S^{xx}(q, \omega)$ and $S^{yy}(q, \omega)$ have been derived using the picture of propagating DWPs. Finally we introduce the use of this model to explain the spin dynamics of CsCoCl₃ taking into account the weak interchain interactions (equation (2)). In section 2, the theory and the results for the eigenvalues of the DWP continuum and DWP bound states are derived. The dynamical spin correlation functions of CsCoCl₃ are presented in section 3. Section 4 contains a discussion of the results obtained.

2. Model and domain wall pair states

The one-dimensional fully anisotropic Ising-like Heisenberg Hamiltonian in the presence of a transverse magnetic field is given by

$$\begin{aligned}
 H &= 2 \sum_i^N [J_x S_i^x S_{i+1}^x + J_y S_i^y S_{i+1}^y + J_z S_i^z S_{i+1}^z] - g_\perp \mu_B H_x \sum_i^N S_i^x \\
 &= 2J \sum_i^N \left[S_i^z S_{i+1}^z + \frac{\epsilon_1}{2} (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) + \frac{\epsilon_2}{2} (S_i^+ S_{i+1}^+ + S_i^- S_{i+1}^-) \right] - h_x \sum_i^N S_i^x
 \end{aligned} \tag{4}$$

where

$$J = J_z \quad \epsilon_1 = \frac{J_x + J_y}{2J} \quad \epsilon_2 = \frac{J_x - J_y}{2J} \quad h_x = g_\perp \mu_B H_x \quad \epsilon_1, \epsilon_2 \ll 1.$$

H_x is the transverse magnetic field and we assume that $h_x \ll 2J$. N is the total number of spins. Since we are interested in excitations at low temperatures, we consider low-lying excited states. These states can be obtained from the Néel state by flipping a block of adjacent spins, giving rise to DWP states with $S_T^z = 0$ and ± 1 (figure 1). These excitations occur around the Ising energy $2J$ above the ground state. Following the method introduced by Murao *et al* [9], we classify these states into two series. Series *a* starts from the state with $S_T^z = 1$ where two domain walls are adjacent. Let m be the number (odd) of sites between two domain walls and $\phi_1^{(a)}(m)$ be the corresponding Ising state. The subsequent states $\phi_j^{(a)}(m)$ ($j = 2, 3, 4, \dots$) are generated from $\phi_1^{(a)}(m)$ such that the separation between the domain walls is increased by unit lattice distance successively towards the right-hand side of the chain. Hence,

$$\begin{aligned}
 \phi_1^{(a)}(m) &= S_m^+ |\text{Néel}\rangle & S_T^z &= 1 \\
 \phi_j^{(a)}(m) &= S_{m+j-1}^- \phi_{j-1}^{(a)}(m) & (j = 2, 4, 6, \dots) & S_T^z = 0 \\
 \phi_j^{(a)}(m) &= S_{m+j-1}^+ \phi_{j-1}^{(a)}(m) & (j = 3, 5, 7, \dots) & S_T^z = 1.
 \end{aligned} \tag{5}$$

$|\text{Néel}\rangle$ is one of the Néel states. We choose a linear combination of these basis states for describing propagating DWPs with wave vector q as

$$|j, q\rangle_a = \sqrt{\frac{2}{N}} \sum_{m=\text{odd}} e^{-iqm} \phi_j^{(a)}(m). \tag{6}$$

On the other hand, series *b* originates from the state with $S_T^z = -1$, and the subsequent states with $S_T^z = 0$ and -1 appear alternately:

$$\begin{aligned}
 \phi_1^{(b)}(m) &= S_m^- |\text{Néel}\rangle & S_T^z &= -1 \\
 \phi_j^{(b)}(m) &= S_{m+j-1}^+ \phi_{j-1}^{(b)}(m) & (j = 2, 4, 6, \dots) & S_T^z = 0 \\
 \phi_j^{(b)}(m) &= S_{m+j-1}^- \phi_{j-1}^{(b)}(m) & (j = 3, 5, 7, \dots) & S_T^z = -1.
 \end{aligned} \tag{7}$$

Taking linear combination of these states with wave vector q ,

$$|j, q\rangle_b = \sqrt{\frac{2}{N}} \sum_{m=\text{even}} e^{-iqm} \phi_j^{(b)}(m). \tag{8}$$

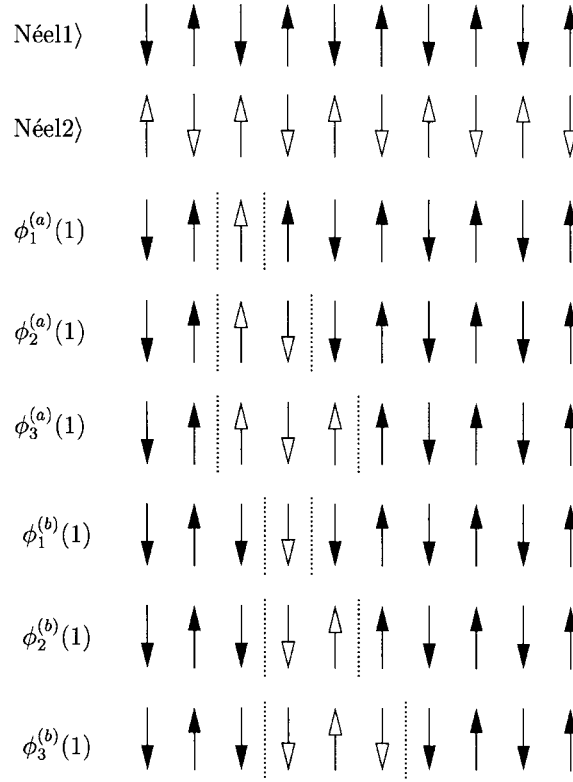


Figure 1. Néel states and DWP states for $S_T^z = \pm 1$ and 0. The dotted vertical lines indicate the positions of domain walls.

With the help of equations (5)–(8), one can obtain $H|j, q\rangle_a$ as follows:

$$\begin{aligned}
 H|1, q\rangle_a &= 2J|1, q\rangle_a + V_{\epsilon_1}|3, q\rangle_a + V_{\epsilon_2}|1, q\rangle_b - \frac{h_x}{2}(|2, q\rangle_a + e^{-iq}|2, q\rangle_b) \\
 H|2, q\rangle_a &= 2J|2, q\rangle_a + V_{\epsilon_1}|4, q\rangle_a - \frac{h_x}{2}(|1, q\rangle_a + |3, q\rangle_a + e^{-iq}|3, q\rangle_b + e^{iq}|1, q\rangle_b) \\
 &\vdots \\
 H|j, q\rangle_a &= 2J|j, q\rangle_a + V_{\epsilon_1}|j+2, q\rangle_a + V_{\epsilon_1}^*|j-2, q\rangle_a - \frac{h_x}{2}(|j-1, q\rangle_a + |j+1, q\rangle_a) \\
 &\quad - \frac{h_x}{2}(e^{iq}|j-1, q\rangle_b + e^{-iq}|j+1, q\rangle_b) \quad j \geq 3
 \end{aligned} \tag{9}$$

where

$$V_{\epsilon_1} = \epsilon_1 J(1 + e^{-2iq}) \quad \text{and} \quad V_{\epsilon_2} = 2\epsilon_2 J \cos q.$$

In the same manner, one could derive a similar set of equations for $H|j, q\rangle_b$ in terms of $|n, q\rangle_a$ and $|n, q\rangle_b$. To avoid the mixing between the states of series a and b , we further introduce symmetric (α) and antisymmetric (β) functions [9] defined as

$$\begin{aligned}
 |j, q\rangle_\alpha &= \frac{1}{\sqrt{2}}(|j, q\rangle_a + |j, q\rangle_b) \\
 |j, q\rangle_\beta &= \frac{1}{\sqrt{2}}(|j, q\rangle_a - |j, q\rangle_b).
 \end{aligned} \tag{10}$$

Hence, one can express $H|j, q\rangle_\alpha$ as

$$\begin{aligned} H|1, q\rangle_\alpha &= (2J + V_{\epsilon_2})|1, q\rangle_\alpha + V_{\epsilon_1}|3, q\rangle_\alpha - V_\alpha|2, q\rangle_\alpha \\ H|2, q\rangle_\alpha &= 2J|2, q\rangle_\alpha + V_{\epsilon_1}|4, q\rangle_\alpha - (V_\alpha^*|1, q\rangle_\alpha + V_\alpha|3, q\rangle_\alpha) \\ &\vdots \\ H|j, q\rangle_\alpha &= 2J|j, q\rangle_\alpha + V_{\epsilon_1}|j+2, q\rangle_\alpha + V_{\epsilon_1}^*|j-2, q\rangle_\alpha - (V_\alpha^*|j-1, q\rangle_\alpha \\ &\quad + V_\alpha|j+1, q\rangle_\alpha) \quad j \geq 3 \end{aligned} \quad (11)$$

where

$$V_\alpha = \frac{h_x}{2}(1 + e^{-iq}).$$

Similarly, one can derive $H|j, q\rangle_\beta$ with α and V_α being replaced by β and

$$V_\beta = \frac{h_x}{2}(1 - e^{-iq})$$

respectively. The first excited states can be constructed as a linear combination of symmetric and antisymmetric functions separately:

$$\Psi_\alpha(q) = \sum_j \alpha_j |j, q\rangle_\alpha \quad \text{and} \quad \Psi_\beta(q) = \sum_j \beta_j |j, q\rangle_\beta. \quad (12)$$

With the help of the equation (11), the following equations for the coefficients α_j and β_j are obtained:

$$\begin{aligned} \lambda_\alpha \bar{\alpha}_1 &= (2J + V_{\epsilon_2})\bar{\alpha}_1 + \bar{V}_\alpha \bar{\alpha}_2 + \bar{V}_{\epsilon_1} \bar{\alpha}_3 \\ \lambda_\alpha \bar{\alpha}_2 &= 2J\bar{\alpha}_2 + \bar{V}_\alpha(\bar{\alpha}_1 + \bar{\alpha}_3) + \bar{V}_{\epsilon_1} \bar{\alpha}_4 \\ &\vdots \\ \lambda_\alpha \bar{\alpha}_j &= 2J\bar{\alpha}_j + \bar{V}_\alpha(\bar{\alpha}_{j-1} + \bar{\alpha}_{j+1}) + \bar{V}_{\epsilon_1}(\bar{\alpha}_{j-2} + \bar{\alpha}_{j+2}) \quad j \geq 3 \end{aligned} \quad (13)$$

where λ_α is the eigenvalue,

$$\bar{V} = -h_x \cos\left(\frac{q}{2}\right)$$

$$\bar{V}_{\epsilon_1} = 2\epsilon_1 J \cos q$$

and

$$\bar{\alpha}_j = \alpha_j e^{(iq/2)j}.$$

In the same manner, one can derive similar set of equations for β with α being replaced by β , \bar{V}_α by

$$\bar{V}_\beta = h_x \sin\left(\frac{q}{2}\right)$$

and $\bar{\alpha}_j$ by

$$\bar{\beta}_j = \beta_j e^{i(k+\pi)/2)j}.$$

Dispersion relations are obtained numerically by solving equations (13), with $N = 1000$. Here, we present the results for $\epsilon_1 = 0.05$ and $\epsilon_2 = 0.10$, since these values are estimated for the compound CsCoCl₃ [11]. Figure 2 shows the dispersion relations in the symmetric and antisymmetric modes, λ_α and λ_β , respectively, for $h_x = 0$. The spin-wave continuum and the bound-state energy are plotted as solid and dotted lines, respectively. In the symmetric mode, the bound-state energy lies above the continuum for $q < \pi/2$ and below the continuum for

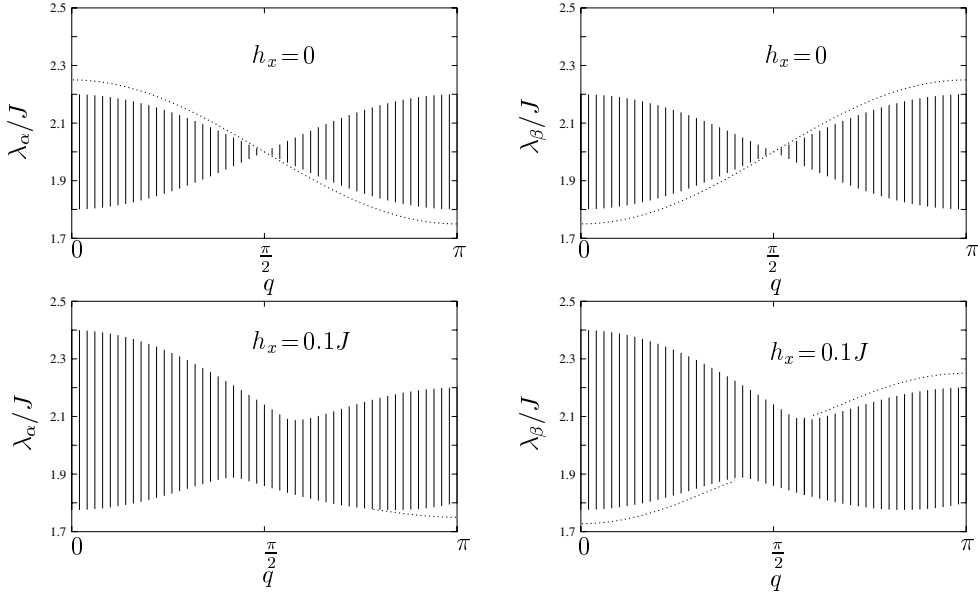


Figure 2. The spin-wave excitation continuum (solid lines) and DWP bound-state energies (dotted lines) of the symmetric and antisymmetric modes for $\epsilon_1 = 0.05$ and $\epsilon_2 = 0.1$.

$q > \pi/2$, while the reverse is true for the antisymmetric mode. The bound state does not exist when $\epsilon_1 > \epsilon_2$. When $h_x \neq 0$, the energy band extends towards the high-energy region for $0 \leq q \leq \pi/2$ in both the symmetric and the antisymmetric modes. The spin-wave excitations have a width at $q = \pi/2$ in contrast with the case for $h_x = 0$. The width also broadens with the increase of h_x . Note that the bound-state energy is not affected by the presence of h_x .

3. Dynamical spin correlation functions at $T = 0$ K

The dynamical spin correlation function along the direction of h_x at $T = 0$ is defined as

$$S^{xx}(q, \omega) = \sum_e |\langle \Psi_e | S^x(q) | \Psi_g \rangle|^2 \delta(\omega - \lambda_e + \lambda_g) \quad (14)$$

where $|\Psi_g\rangle$, $|\Psi_e\rangle$ denote the ground and excited states, respectively, and λ_g, λ_e are the corresponding eigenvalues. In this case, the ground state is one of the Néel states and the summation extends over the first excited states only. Also

$$S^x(q) = \frac{1}{2\sqrt{N}} \sum_j e^{iqr_j} (S_j^+ + S_j^-).$$

Similarly, the dynamical spin correlation function perpendicular to the direction of h_x , $S^{yy}(q, \omega)$, is defined by replacing the superscript x with y in equation (14), where

$$S^y(q) = \frac{1}{2i\sqrt{N}} \sum_j e^{iqr_j} (S_j^+ - S_j^-).$$

Since the ground state is the Néel state, $S^{xx}(q, \omega)$ and $S^{yy}(q, \omega)$ directly reflect the wavenumber dependence of the excited states.

With the help of the equation (12), the dynamical spin correlation functions can further be written as [9]

$$\begin{aligned} S^{xx}(q, \omega) &= \frac{1}{4} \sum_{\alpha} |\alpha_1|^2 \delta(\omega - \lambda_{\alpha} + \lambda_g) \\ S^{yy}(q, \omega) &= \frac{1}{4} \sum_{\beta} |\beta_1|^2 \delta(\omega - \lambda_{\beta} + \lambda_g). \end{aligned} \quad (15)$$

Note that $S^{xx}(q, \omega)$ depends only depends on $|\alpha_1|^2$ while $S^{yy}(q, \omega)$ depends on $|\beta_1|^2$. Thus, the symmetric mode is directly reflected in $S^{xx}(q, \omega)$, whereas the antisymmetric mode is reflected in $S^{yy}(q, \omega)$. The functions $S^{xx}(q, \omega)$ and $S^{yy}(q, \omega)$ for $h_x = 0$ are shown in figure 3. A sharp peak originates from the bound state, whereas the broad peak originates from the free DWP states. The intensity of the sharp peak does not depend on the number of spins N , while the broad peak comprises $N - 1$ peaks which have intensity of the order of $1/N$. Note that at the zone boundary ($q = \pi/2$), the width of the continuum vanishes. This is also verified in neutron scattering experiments on CsCoCl₃ [12].

The line shapes of $S^{xx}(q, \omega)$ at $h_x = 0.1J$ have been plotted in figure 4. The main feature of $S^{xx}(q, \omega)$ induced by h_x shows that the line shape is purely symmetric at the zone boundary

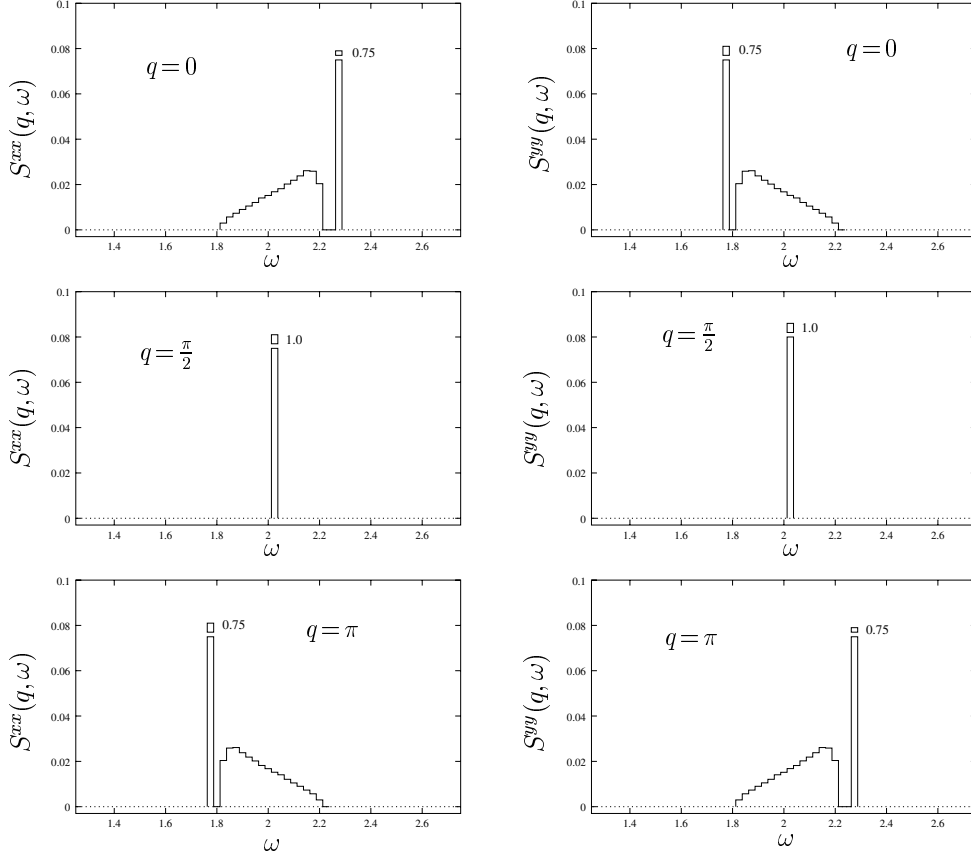


Figure 3. The functions $S^{xx}(q, \omega)$ and $S^{yy}(q, \omega)$ for $q = 0, \pi/2$ and π in histograms with $\Delta\omega = 0.025J$.

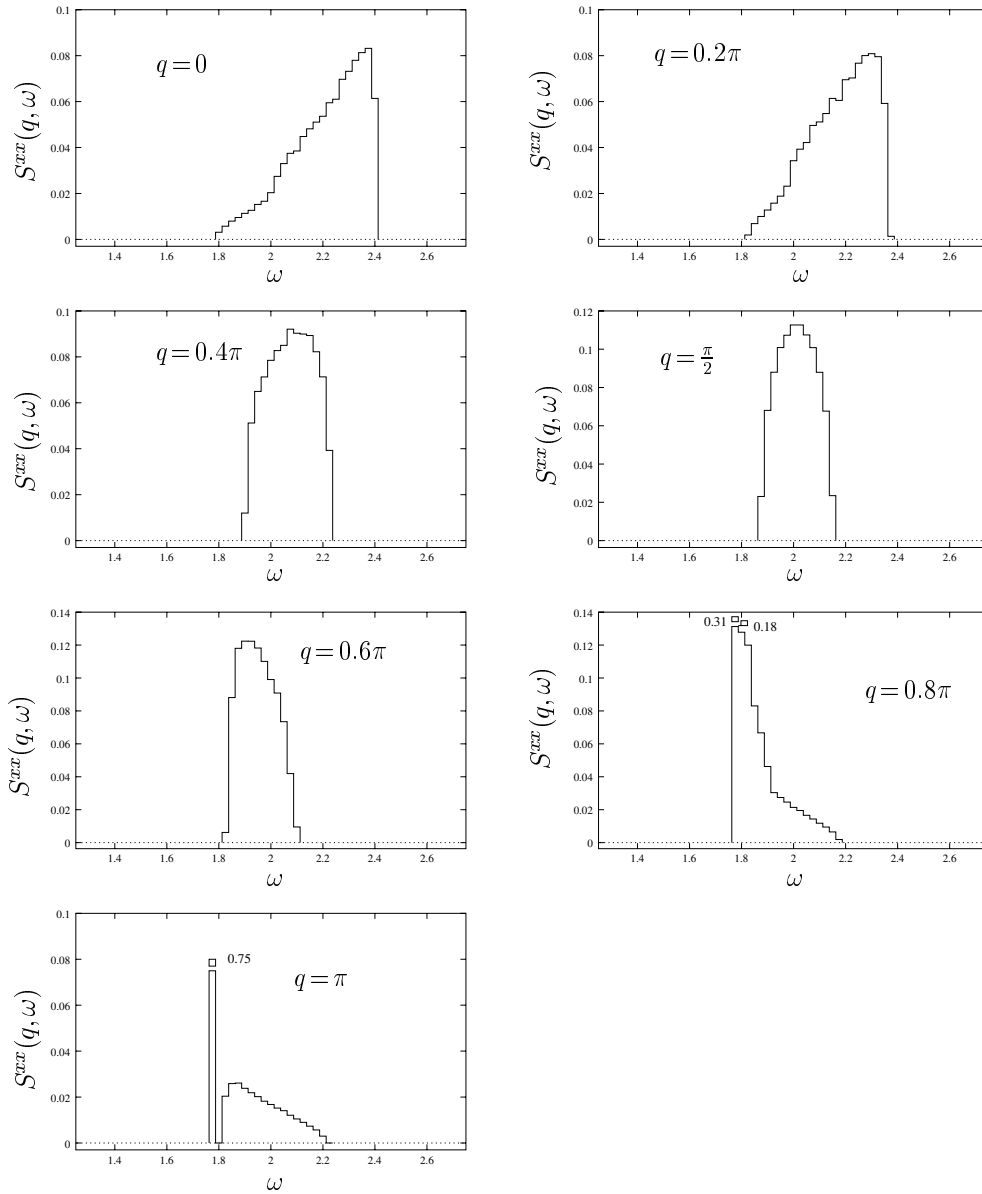


Figure 4. The function $S^{xx}(q, \omega)$ for different values of q and $h_x = 0.1J$. The width of each histogram is $\Delta\omega = 0.025J$.

and it is highly asymmetric away from the zone boundary. At $q \approx 0$, the sharp peak occurs at high energy and the tail in the lower-energy region. For $0 < q < \pi/2$, the spectral weight concentrates mainly in the middle of the continuum. The sharp peak emerges again in the lower-energy region for $\pi/2 < q < \pi$. At $q \approx \pi$, the line shape is not affected by h_x as expected from the dispersion relation shown in figure 2.

Figure 5 shows $S^{yy}(q, \omega)$ at $h_x = 0.1J$. The line shape of $S^{yy}(q, \omega)$ is again symmetric at $q = \pi/2$. The q -dependence of $S^{yy}(q, \omega)$ is opposite to that of $S^{xx}(q, \omega)$ and it remains

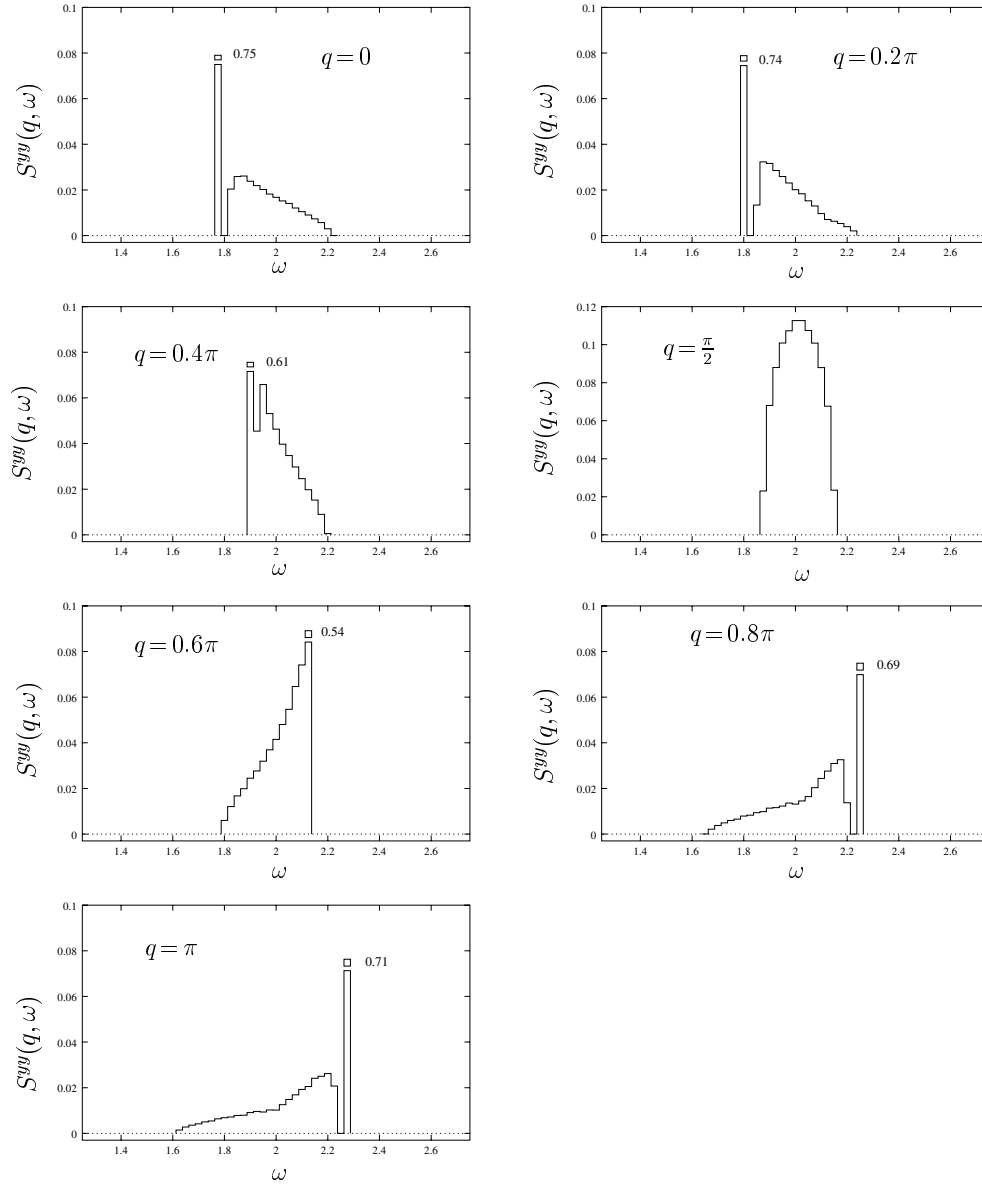


Figure 5. The function $S^{yy}(q, \omega)$ for different values of q and $h_x = 0.1J$. The width of each histogram is $\Delta\omega = 0.025J$.

unaffected at $q = 0$. For $0 < q < \pi/2$, the sharp peak appears in the lower-energy region of the broad peak. The sharp peak originates from the bound state, whereas the broad peak originates from the DWP continuum. For $\pi/2 < q < \pi$, the sharp peak appears on the higher-energy side of the broad peak and the tail is found to be enhanced towards the lower-energy region.

In figures 6 and 7, $S^{xx}(q, \omega)$ and $S^{yy}(q, \omega)$ are shown for different values of h_x , respectively. With the increase of h_x , the features mentioned above are enhanced. The

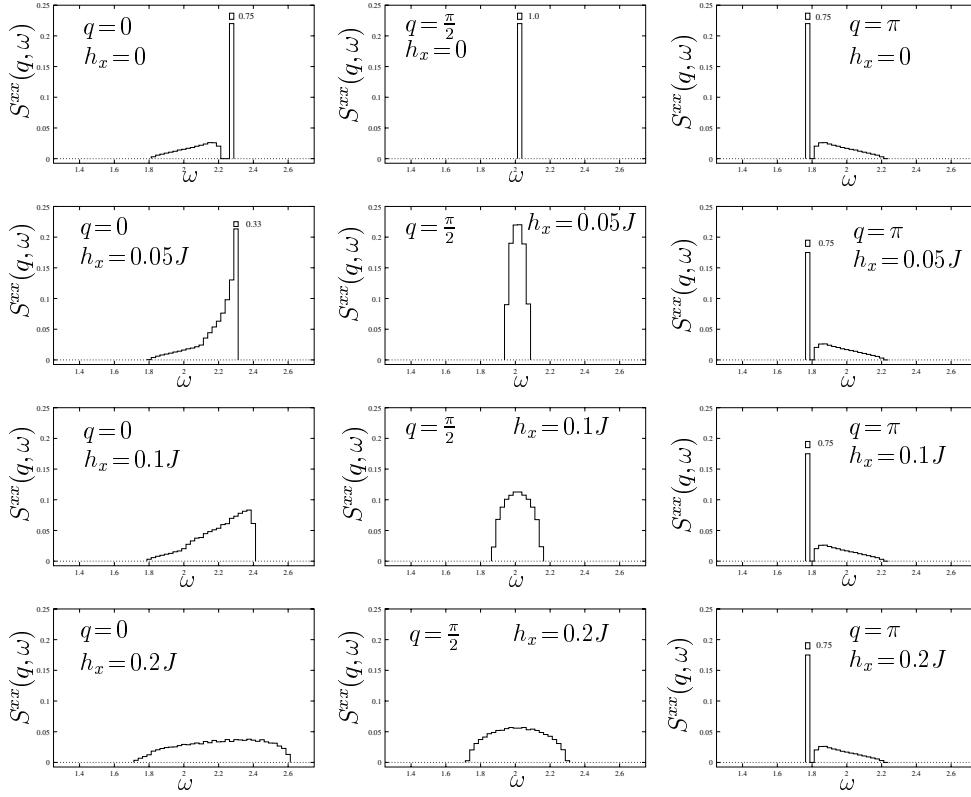


Figure 6. The function $S^{xx}(q, \omega)$ for different values of q and h_x . The width of each histogram is $\Delta\omega = 0.025J$.

height of the sharp peak is found to diminish with the increase of h_x . Note that $S^{xx}(q, \omega)$ for $0 < q < \pi/2$ and $S^{yy}(q, \omega)$ for $\pi/2 < q < \pi$ are sensitive to h_x as observed by Murao *et al* [9].

3.1. Interchain interactions in CsCoCl_3

Now we add the staggered-field term to the Hamiltonian in equation (5). The full Hamiltonian looks as follows:

$$H = 2J \sum_i^N \left[S_i^z S_{i+1}^z + \frac{\epsilon_1}{2} (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) + \frac{\epsilon_2}{2} (S_i^+ S_{i+1}^+ + S_i^- S_{i+1}^-) \right] - h_x \sum_i^N S_i^x - h_{ic} \sum_i^N (-1)^i S_i^z. \quad (16)$$

Here, we further consider that the staggered field h_{ic} originates due to the weak interchain interaction. The interchain interaction has been treated in the mean-field approximation. Thus,

$$h_{ic} = 2J' \sum_{\delta} \langle S_{i+\delta}^z \rangle \quad (17)$$

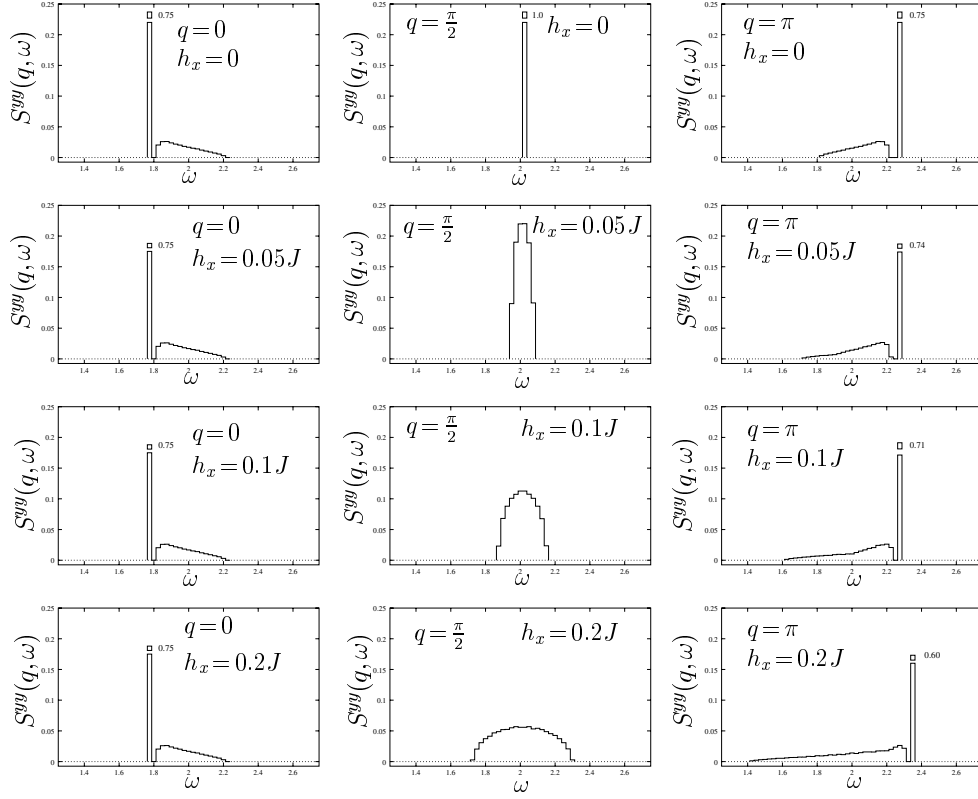


Figure 7. The function $S^{yy}(q, \omega)$ for different values of q and h_x . The width of each histogram is $\Delta\omega = 0.025J$.

where J' is the interchain interaction strength and δ is the nearest neighbour on the ab -plane. Following the same technique as was developed in section 2, we obtain $S^{xx}(q, \omega)$ and $S^{yy}(q, \omega)$ numerically.

In figure 8, $S^{xx}(q, \omega)$ is shown for different values of h_{ic} . When $h_{ic} \neq 0$, the broad peak of $S^{xx}(q, \omega)$ has been split into discrete peaks, which are known as the Zeeman ladder [13]. With the increase of h_{ic} , the number of peaks decreases and the separation between them becomes wider. For $\pi/2 < q < \pi$, the intensity of the peak at the lowest energy is stronger. Several peaks having nearly the same intensity are observed at $q \approx 0$.

Figure 9 shows $S^{yy}(q, \omega)$ for different values of h_{ic} . For $0 \leq q \leq \pi/2$, several strong peaks appear in the lower-energy region. Note that the differences between $S^{xx}(q, \omega)$ and $S^{yy}(q, \omega)$ are remarkable at $q = \pi$. In $S^{yy}(q, \omega)$ for $q = \pi$, several strong peaks appear in the higher-energy region and weak peaks in the lower-energy region, and their intensities vary irregularly with the increase in h_{ic} . Thus the combined effect of h_x and the interchain interactions is also found in $S^{xx}(q, \omega)$ and $S^{yy}(q, \omega)$ for $q \geq \pi/2$ as reported in reference [9].

In CsCoCl_3 , the magnetic Co^{2+} ions are surrounded by trigonally distorted octahedra of Cl^- ions and form chains along the c -axis with successive octahedra sharing a common face. The CsCl_3^- chains are arranged in a triangular array. Since the exchange coupling between chains is antiferromagnetic, the triangular array forms a frustrated system. Thus there is no possibility of a perfectly regular AFM ordered state. Two different three-dimensionally ordered phases occur in CsCoCl_3 . First, below $T_{N_1} \sim 21$ K a partially disordered AFM phase (A) is

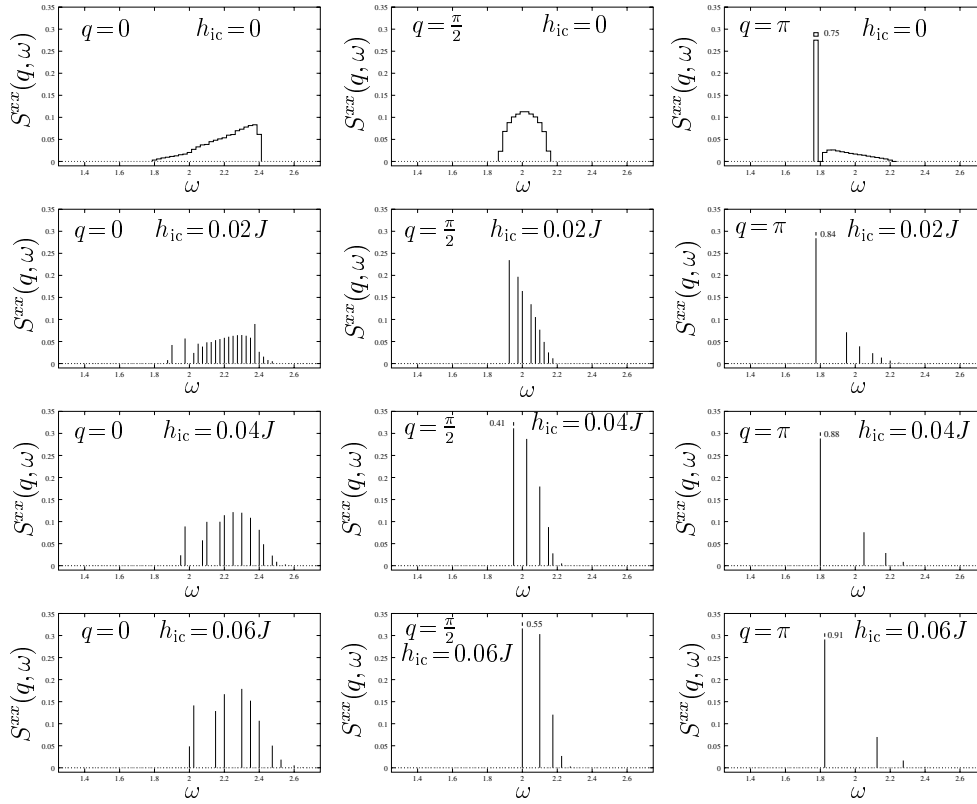


Figure 8. The function $S^{xx}(q, \omega)$ for different values of h_{ic} and $h_x = 0.1J$. The width of each histogram is $\Delta\omega = 0.025J$.

formed in which a third of the chains are paramagnetic. A phase change takes place below $T_{N_2} \sim 10\text{--}14$ K, to a ferrimagnetic phase (F), in which the paramagnetic chains align in the same direction, with the result that two thirds of the chains are aligned in one direction and one third in the opposite direction (figure 10) [14].

It is obvious from equation (17) that the staggered field h_{ic} could take one of the two possible values $h_{ic} = 6J'$ and 0. Similarly, in the partially disordered phase, h_{ic} takes one of the four values $h_{ic} = 6J', 4J', 2J'$ and 0. The functions $S^{xx}(q, \omega)$ and $S^{yy}(q, \omega)$ of CsCoCl_3 are obtained by summing those of the individual chains. In the ferrimagnetic phase, the ratio of the numbers of chains with $h_{ic} = 6J'$ and 0 is estimated as 1:2. In the partially disordered phase, the ratio of the numbers of chains with $h_{ic} = 6J', 4J', 2J'$ and 0 is estimated as 1:3:3:5 [9]. Figure 11 shows $S^{xx}(q, \omega)$ for $q = 0$ and $S^{yy}(q, \omega)$ for $q = \pi$ in the ferrimagnetic phase. The line shape of $S^{xx}(q, \omega)$ is affected strongly by h_x . As h_x increases, the differences in intensities among various discrete peaks reduce markedly and the sharp peak disappears. On the other hand, $S^{yy}(q, \omega)$ is affected only slightly by h_x . The spectral weight is enhanced towards the lower-energy region with the increase in h_x , and the intensity distribution varies irregularly. $S^{xx}(q, \omega)$ for $q = 0$ and $S^{yy}(q, \omega)$ for $q = \pi$ obtained in the partially disordered phase are shown in figure 12. $S^{xx}(q, \omega)$ is strongly affected by h_x while $S^{yy}(q, \omega)$ is much less affected. $S^{xx}(q, \omega)$ for $q = \pi$ and $S^{yy}(q, \omega)$ for $q = 0$ are not affected by h_x in either the ferrimagnetic or the partially disordered phases.

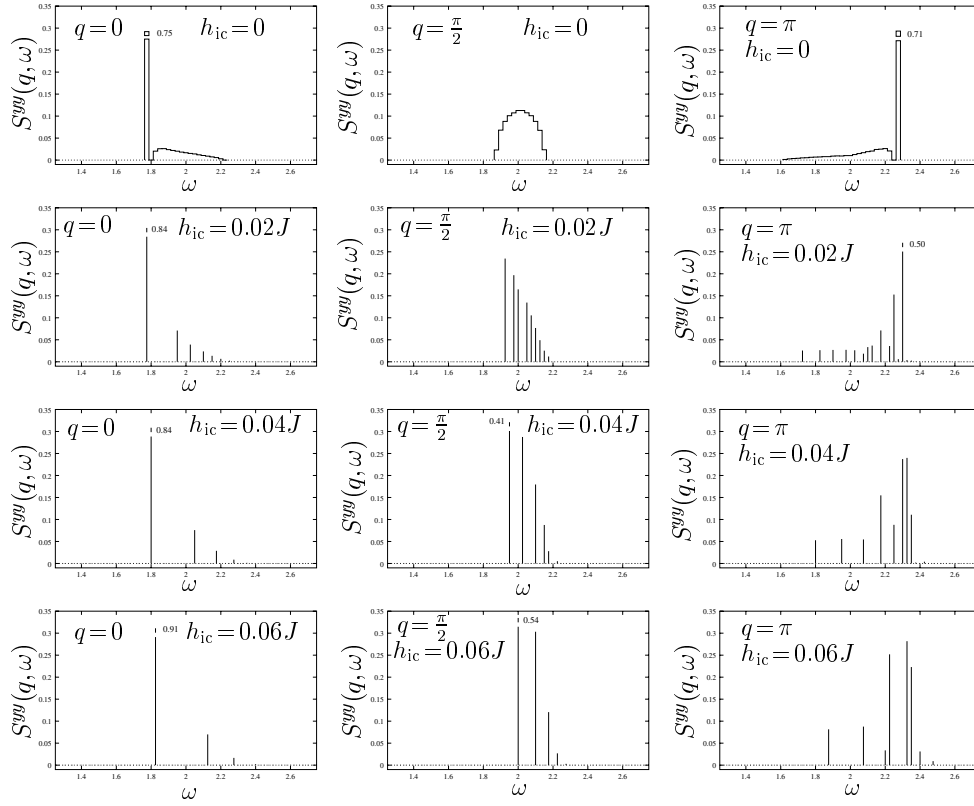


Figure 9. The function $S^{yy}(q, \omega)$ for different values of h_{ic} and $h_x = 0.1J$. The width of each histogram is $\Delta\omega = 0.025J$.

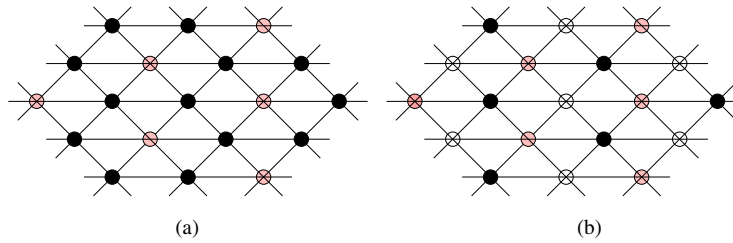


Figure 10. Magnetic ordering in the ab -plane below T_{N1} : (a) ferrimagnetic structure for $T < T_{N2}$ (F phase); (b) structure for $T_{N2} < T < T_{N1}$ (A phase). Chains marked with open circles are disordered.

4. Discussion of results

We have studied the effect of the transverse magnetic field h_x on dynamical properties of the one-dimensional fully anisotropic Ising-like antiferromagnet at low temperatures. We have shown using this Hamiltonian that some of the results obtained by Murao *et al* in [9], where a FM NNN interaction is assumed besides the usual AFM NN interaction, can be qualitatively reproduced. These include the formation of DWP bound states, two types of excited mode which are symmetric and antisymmetric with respect to the states with $S_T^z = 1$ and -1 and

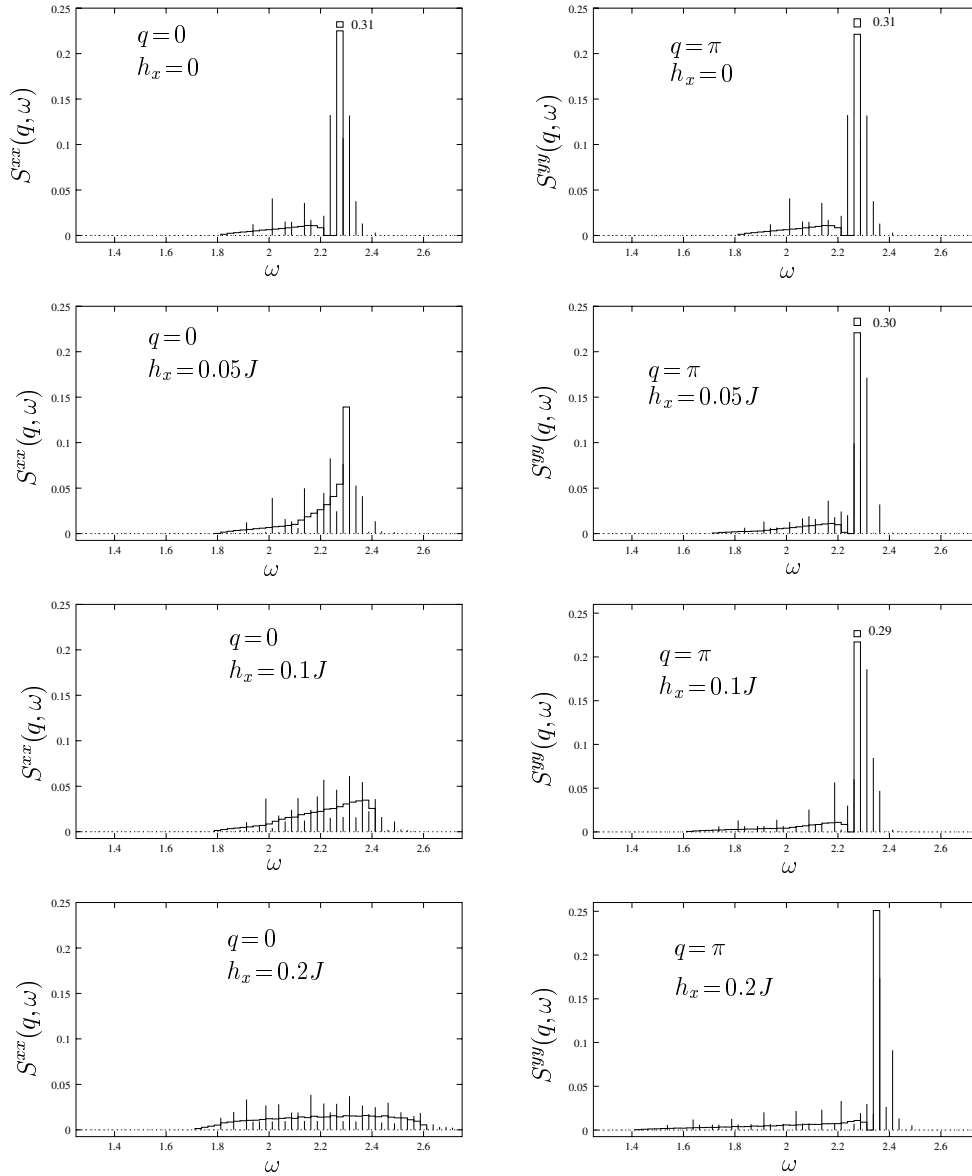


Figure 11. The function $S^{xx}(q, \omega)$ for $q = 0$ and $S^{yy}(q, \omega)$ for $q = \pi$ in the ferrimagnetic phase. The width of each histogram is $\Delta\omega = 0.025J$.

an asymmetry in the line shapes of the correlation functions $S^{xx}(q, \omega)$ and $S^{yy}(q, \omega)$. In order to obtain the asymmetry in the line shapes of $S^{xx}(q, \omega)$ and $S^{yy}(q, \omega)$, a FM NNN exchange of magnitude $|J'| \sim 0.1|J|$ is required, which, considering that the NNN exchange is through two nonmagnetic ligands, would seem to be unphysically large [10]. On the other hand, our model could explain all of these characteristics with the usual NN AFM exchange interactions. There are, however, a number of differences. Murao *et al* [9] observed a single bound-state branch which is symmetric with respect to the zone boundary, whereas in the present study, different bound-state branches are obtained for symmetric and antisymmetric

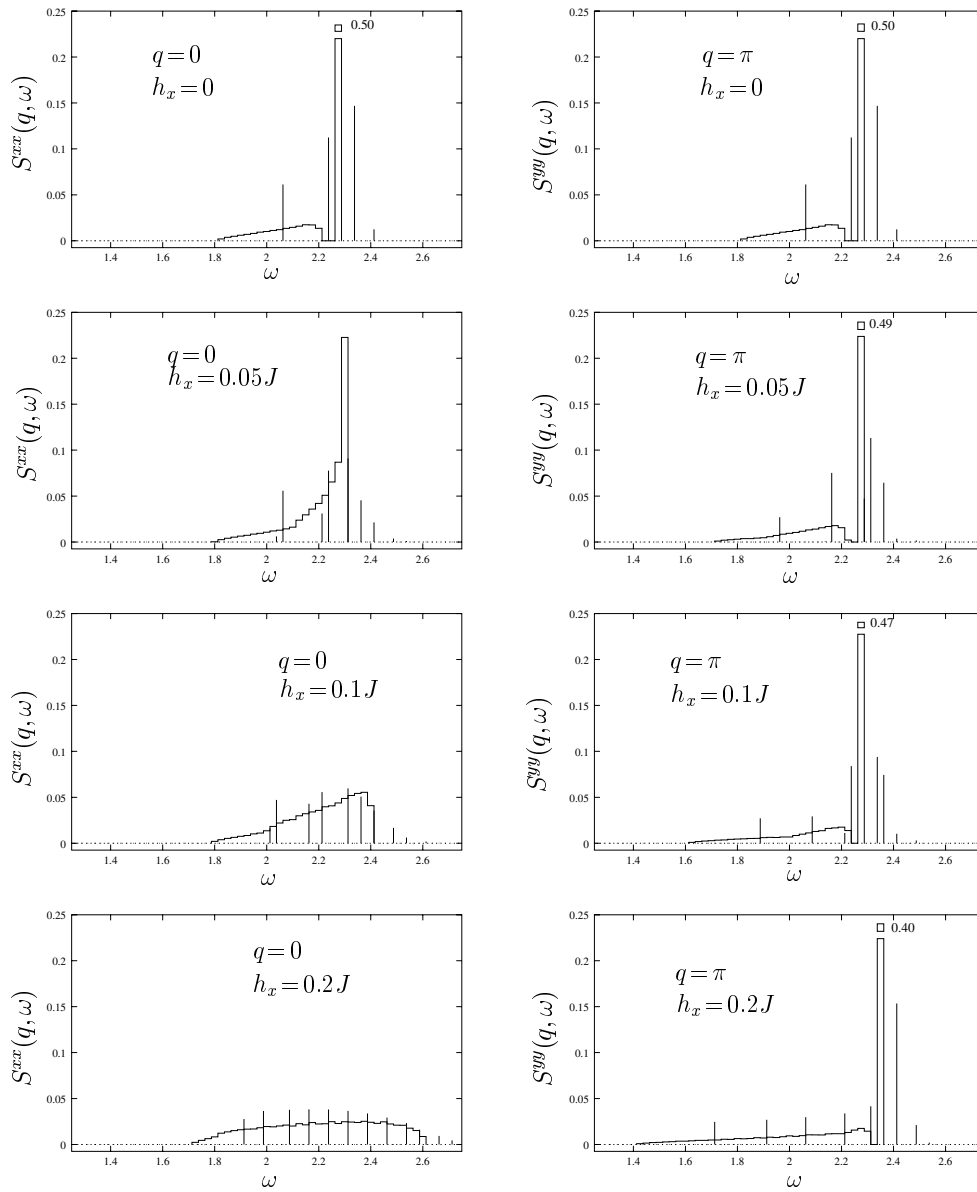


Figure 12. The function $S^{xx}(q, \omega)$ for $q = 0$ and $S^{yy}(q, \omega)$ for $q = \pi$ in the partially disordered phase. The width of each histogram is $\Delta\omega = 0.025J$.

modes which are asymmetric with respect to the zone boundary. No experimental evidence is as yet available on the effect of bound states on the thermodynamic and dynamic properties of the compounds CsCoCl_3 and CsCoBr_3 . The symmetric modes contribute to $S^{xx}(q, \omega)$, whereas antisymmetric modes contribute to $S^{yy}(q, \omega)$. Both $S^{xx}(q, \omega)$ and $S^{yy}(q, \omega)$ have symmetry at the zone boundary even in the presence of either (i) both h_x and h_{ic} or (ii) either one of them. This symmetry is totally lost away from the zone boundary. This theory is also valid for analysis of the spin dynamics of CsCoCl_3 and CsCoBr_3 at finite temperatures, because

the correlation length of the spin along the chain is very large even in the paramagnetic phase ($T \approx 21$ K). Thus the effects of h_x on $S^{xx}(q, \omega)$ and $S^{yy}(q, \omega)$ discussed here are yet to be observed in a real system.

Apart from the relevance to experimental systems such as CsCoCl_3 and CsCoBr_3 , the present study is intended to provide insights into the spin dynamics of the fully anisotropic Ising-like AFM system in the presence of a transverse magnetic field h_x . The ground-state energy and low-lying excitation spectrum of the fully anisotropic Hamiltonian are known exactly because of the mapping between the fully anisotropic Hamiltonian and the exactly solvable eight-vertex model [15, 16]. Our calculations provide us with some physical insights into the spin dynamics in an Ising-like fully anisotropic AFM system in the presence of a transverse magnetic field.

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