Optical absorption of $S = 1/2$ two-leg spin ladder systems

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Abstract

We calculate the optical absorption spectrums for the $S = 1/2$ two-leg spin ladder systems using continued fraction method based on Lanczos algorithm. We use two sets of parameters suggested for a $S = 1/2$ two-leg spin ladder material $SrCu_2O_3$. We find that due to a cyclic four-spin interaction the dispersion curve becomes flatter and hence the large peak structure appears in the optical absorption spectrums.

Key words: optical absorption spectrums; $S = 1/2$ two-leg spin ladder; cyclic four-spin interaction; $SrCu_2O_3$

$S = 1/2$ two-leg spin ladder systems with antiferromagnetic interactions have been studied intensively [1]. Fascinating aspects of the elementary excitation as well as thermodynamic properties have been revealed. Recently, the $S = 0$ two-magnon bound state as well as excitation continuum was observed by the optical absorption spectrums for an $S = 1/2$ two-leg spin ladder material $(Ca, La)_{14}Cu_{24}O_{41}$ [2]. For $SrCu_2O_3$, which is an $S = 1/2$ two-leg spin ladder material, two sets of parameters were proposed to reproduce temperature dependence of the susceptibility [3,4]. Note that in one set of parameters importance of a cyclic four-spin interaction has been pointed out [3]. It may be difficult to decide the proper model only from temperature dependence of the susceptibility.

In this paper, we calculate the optical absorption spectrums for $S = 1/2$ two-leg spin ladder systems using two sets of parameters for $SrCu_2O_3$. Let us consider the following Hamiltonian,

$$\begin{aligned} H = & J_{\parallel} \sum_{i=1}^{N/2} (\boldsymbol{S}_{1,i} \cdot \boldsymbol{S}_{1,i+1} + \boldsymbol{S}_{2,i} \cdot \boldsymbol{S}_{2,i+1}) \\ & + J_{\perp} \sum_{i=1}^{N/2} \boldsymbol{S}_{1,i} \cdot \boldsymbol{S}_{2,i} \\ & + J_{cyc} \sum_{i=1}^{N/2} \{4[(\boldsymbol{S}_{1,i} \cdot \boldsymbol{S}_{1,i+1})(\boldsymbol{S}_{2,i+1} \cdot \boldsymbol{S}_{2,i}) + (\boldsymbol{S}_{1,i} \cdot \boldsymbol{S}_{2,i}) \\ & \times (\boldsymbol{S}_{1,i+1} \cdot \boldsymbol{S}_{2,i+1}) - (\boldsymbol{S}_{1,i} \cdot \boldsymbol{S}_{2,i+1})(\boldsymbol{S}_{1,i+1} \cdot \boldsymbol{S}_{2,i})] \\ & + (\boldsymbol{S}_{1,i} \cdot \boldsymbol{S}_{1,i+1}) + (\boldsymbol{S}_{1,i+1} \cdot \boldsymbol{S}_{2,i+1}) \\ & + (\boldsymbol{S}_{2,i+1} \cdot \boldsymbol{S}_{2,i}) + (\boldsymbol{S}_{2,i} \cdot \boldsymbol{S}_{1,i}) + \frac{1}{4}\} \\ & + J_{diag} \sum_{i=1}^{N/2} (\boldsymbol{S}_{1,i} \cdot \boldsymbol{S}_{2,i+1} + \boldsymbol{S}_{1,i+1} \cdot \boldsymbol{S}_{2,i}) , \end{aligned} \tag{1}$$

where $\boldsymbol{S}_{l,i}$ denotes the $S = 1/2$ spin operator in the i-th rung of the $l = 1, 2$ chain, N is the total number of the site, and $J_{\parallel}$ and $J_{\perp}$ are the coupling constants for the interactions along the leg and rung, respectively. J_{cyc} and J_{diag} are the coupling constants for a cyclic four-spin interaction and a diagonal interaction, respectively. Two sets of parameters for $SrCu_2O_3$ are, (a) $J_{\perp} = 150$meV, $J_{\parallel} = 195$meV, $J_{cyc} = 18$meV and $J_{diag} = 3$meV [3], and (b) $J_{\perp} = 86$meV, $J_{\parallel} = 172$meV [4].

Using continued fraction method based on Lanczos algorithm, we calculate the optical absorption spectrums defined as

$$I(\omega) = -\frac{1}{\pi} \int d\boldsymbol{q} \mathrm{Im} \langle \phi_o | R(\boldsymbol{q})^{\dagger} \frac{1}{\omega - H + i0^{+}} R(\boldsymbol{q}) | \phi_o \rangle, \tag{2}$$

where $|\phi_o\rangle$ is the eigenfunction of the ground state and

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$\boldsymbol{q}$= (q_x, q_y) with the wave numbers along the leg (q_x) and the rung ($q_y = 0, \pi$). For the polarization along the leg and the rung, $I(\omega)$ is given by the contributions $R_l(q_x, q_y) = (1/\sqrt{N}) \sum_{i,j} \boldsymbol{S}_{j,i} \cdot \boldsymbol{S}_{j,i+1} e^{i(q_x i + q_y j)}$ and $R_r(q_x) = (\sqrt{2/N}) \sum_i \boldsymbol{S}_{1,i} \cdot \boldsymbol{S}_{2,i} e^{i q_x i}$, respectively.

First, we calculate the $\boldsymbol{q}$-resolved optical absorption spectrums. The results are shown in Fig. 1. Note that the energy is measured in units of $J_\parallel$. The intensity is proportional to the area of the circle. In the leg polarization, the largest intensity for given q_x lies in the lowest excited state. In the rung polarization, on the contrary, the largest intensity for some q_x lies not in the lowest excited state but in the higher excited state. The solid lines denote the dispersion relation of the lowest excited states. In the leg polarization, the dispersion relations of the parameter (a) become flatter than those of the parameter (b). This tendency becomes noticeable for $q_y = 0$. The flat dispersion relation may be caused by the effect of a cyclic four-spin interaction.

By integrating each result in Fig.1 with respect to $\boldsymbol{q}$, the optical absorption spectrums along the leg polarization and the rung polarization for $N = 24$ can be obtained. The results are shown in Fig. 2. The optical absorption spectrums along the leg polarization provide the dominant contribution. In the leg polarization for the parameter (a), the sharp peak structure appears at $\omega \sim 1.4$, which originates from the flat dispersion relation with $1.3 < \omega < 1.5$ for $q_y = 0$ mode of the parameter (a). Such a large peak is detectable by phonon-assisted optical absorption experiments [2,5,6]. The experimental findings may be effective to decide the minimal model for $SrCu_2O_3$.

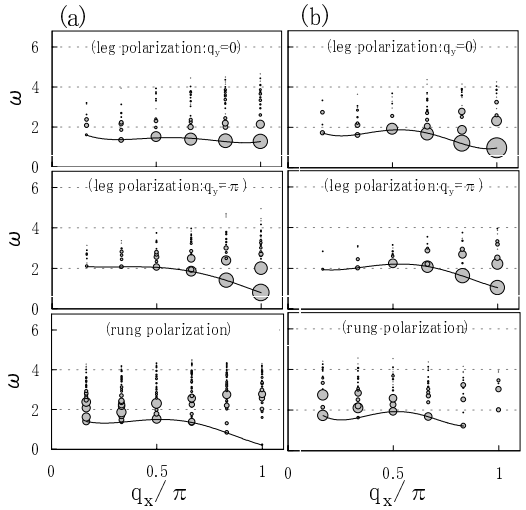

Fig. 1. $\boldsymbol{q}$-resolved optical absorption spectrums. Parameters used are (a) $J_\perp/J_\parallel = 0.769$, $J_{cyc}/J_\parallel = 0.0923$, and $J_{diag}/J_\parallel = 0.0154$, and (b) $J_\perp/J_\parallel = 0.5$, $J_{diag}/J_\parallel = J_{cyc}/J_\parallel = 0.0$, which correspond to those proposed in Refs. 3 and 4, respectively.

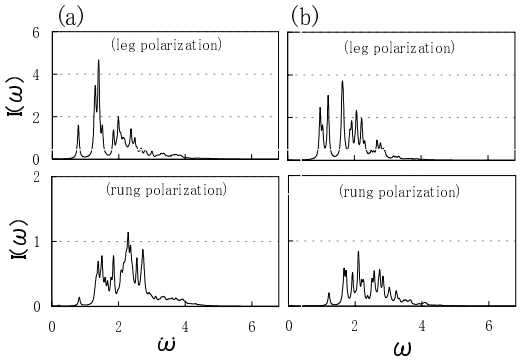

Fig. 2. The optical absorption spectrums along the leg and the rung polarizations. The parameters in (a) and (b) are corresponding to those of Fig. 1 (a) and (b), respectively.

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