Enhancement of the Thermal Conductivity in the spin-Peierls system

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Abstract

We study mechanism of magnetic energy transport, motivated by recent measurements of the thermal conductivity in low dimensional quantum magnets. We point out a possible mechanism of enhancement of the thermal conductivity in spin-Peierls system, where the magnetic energy transport plays a crucial role. This mechanism gives an interpretation for the recent experiment of $CuGeO_3$.

Key words: Quantum Magnetism; Spin-peierls system;Thermal Conductivity

1. Introduction

The relationship of the thermal conductivity and magnetic state in various low dimensional quantum magnets has been attracted interests [1]. Unusual enhancement of conductivity is observed at low temperatures below a spin gap temperature in gapped spin system such as the two-dimensional dimer spin system $SrCu_2(BO_3)_2$, and the ladder system (Sr, Ca)$_{14}Cu_{24}O_{41}$. This enhancement was usually attributed to the contribution of phononic energy transport.

Recently Hofmann et al. compared the properties of thermal conductivity of $SrCu_2(BO_3)_2$ and $CuGeO_3$ [2]. They investigated the thermal conductivity along different crystal axes, to clarify whether the enhancement of the thermal conductivity is caused by phonons or not. In $SrCu_2(BO_3)_2$, they found that the phononic energy transport is dominant by the observation that the thermal conductivity does not depend on the crystal direction. On the other hand, they found that $CuGeO_3$ shows the direction dependence of thermal conductivity.

Motivated by these recent experiments, we theoretically investigate the role of magnetic transport when the system has the energy gap, and propose a mechanism of enhancement of the thermal conductivity in magnetic systems. We consider a bond-alternating antiferomagnetc Heisenberg chain, and investigate the thermal conductivity focusing on the dependence on the energy gap. Our study is consistent with Hofmann's recent experiments [2].

2. Model and Results

The system we shall consider is an alternate Heisenberg spin chain described by,

$$H = J \sum_{\ell=1}^{N-1} \left(1 - (-1)^{\ell} \delta\right) \mathbf{S}_{\ell} \cdot \mathbf{S}_{\ell+1}, \tag{1}$$

where J is an exchange interaction which is taken as a unity throughout this paper, and $\mathbf{S}_\ell$ is the ℓth spin. The number of spins N is taken to be even. A finite value of parameter δ causes a bond-alternation, which yields the dimerized ground state and a finite spin gap. We study the thermal conductivity for various values of δ. It is difficult to treat the Green-Kubo formula nu-

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merically because it requires infinite N. Therefore the quantum master equation approach is more tractable in numerical simulations. We study the spin system which is directly connected to the reservoirs of different temperatures at the ends using master equation (e.g., see the reference [4] and references therein). We here consider a system of $N = 8$. Although this lattice size is small, we believe that the essential mechanism of magnetic energy transport is clarified. We define the thermal conductivity by measuring the stationary energy current setting

$$T_{\mathrm{R}} = T_{\mathrm{L}} + \Delta T, \tag{2}$$

where T_{L} and T_{R} are the temperatures of left and right reservoir. ΔT is a temperature difference between two reservoirs, and is taken as $\Delta T = 0.3$. Thereby the thermal conductivity $\kappa(T)$ is defined as

$$\kappa(T = T_{\mathrm{L}}) = \frac{\mathrm{Tr}\left(\hat{J}\rho_{\mathrm{st}}\right)}{\Delta T}, \tag{3}$$

where $\hat{J}$ is the total current operator $\hat{J}$ for (1) which is calculated by the continuity equation of the energy as $\hat{J} = -J\left(1-\delta^2\right)\sum_{\ell=1}^{N-2}\left(\mathbf{S}_\ell \times \mathbf{S}_{\ell+1}\right)\cdot \mathbf{S}_{\ell+2}$

We present the results of the thermal current $\kappa(T)\Delta T$ normalized by $N-2$. In Fig.1, the normalized thermal currents are shown for $N = 8$. In the inset, the data of the specific heat are also shown. In the isotropic case, $\delta = 0$, the overall form of the thermal conductivity is similar to that obtained by Klümper and Sakai who exactly calculated the amplitude of zero frequency contribution in the Green-Kubo formula [5]. That is, the thermal conductivity has one peak at about $T \sim 0.5$. This behavior is a common characteristic which does not change when the system size increases. At very low temperatures $\kappa(T)$ should be in proportional to T due to the temperature dependence of specific heat, which is similar to the Casimir's theory in phononic transport [6]. This low temperature property, however, cannot be checked for such finite sizes. We must note that even in the isotropic case $\delta = 0$, the system has a finite energy gap due to the finite size effect. When δ becomes finite, the gap increases, e.g., in the case of $N = 8$, $\Delta E = 0.39269, \Delta E = 0.74750, 1.09041, 1.41106, 1.71290,$ and 1.85807 for $\delta = 0.0, 0.2, 0.4, 0.6, 0.8,$ and 0.9, respectively.

Small bond alternations enhance the thermal conductivity in spite that the alternation tends to separate the system into local spin pairs. This enhancement is observed for even $\delta = 0.8$, and this feature is quite robust. In the case of very large δ, the thermal conductivity is reduced due to the effect of separation of the system. The temperature of the peak of thermal conduction roughly corresponds to half of energy gap like the Shotky-type specific heat. Actually the overall behavior of thermal conductivity is similar to that of the

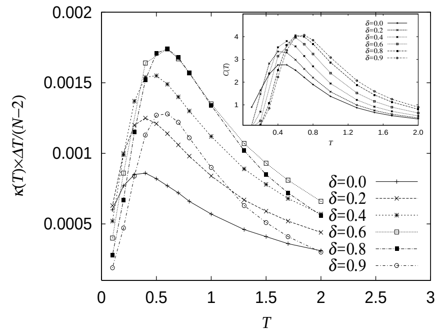

Fig. 1. The thermal conductivities for various δ with the system size $N = 8$. The inset is the specific heat.

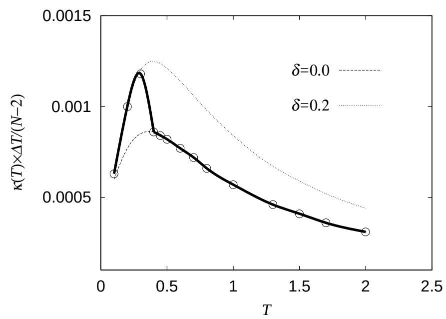

Fig. 2. Demonstration of enhancement of thermal conductivity system size $N = 8$.

specific heat. Thus from this observation, we conclude that the mean free path does not drastically changed by the bond-alternation. We expect that the unusual enhancement of the thermal conductivity in the spin-Peierls system is caused by magnetic energy transport when T_{SP} is the same order of ΔE. In $CuGeO_3$, T_{SP} is the same order of ΔE, i.e., $T_{\mathrm{SP}} \sim 14K$ and $\Delta E \sim 20K$. We demonstrate the enhancement of thermal conductivity below T_{SP} assuming $T_{\mathrm{SP}} = 0.4$ in Fig.2. This figure is similar to the recent experiment of thermal conductivity in $CuGeO_3$ [2].

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