Anomalous spin excitations in a coupled spin-pseudospin model for anisotropic Hubbard ladders at quarter filling

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Abstract

By using the quantum Monte Carlo and density-matrix renormalization group methods, we study the coupled spin-pseudospin Hamiltonian in one-dimension (1D) that models the charge-ordering instability of the anisotropic Hubbard ladder at quarter filling in a strong coupling limit. We here present the temperature dependence of the specific heat of the system to clarify consequences of the interplay between its spin and charge degrees of freedom. We show that there is a parameter and temperature region where the spin degrees of freedom are separated from the charge degrees of freedom and behave like a 1D antiferromagnetic Heisenberg model.

Key words: charge ordering; α'-NaV_2O_5; Hubbard ladder; quarter filling; pseudospin

1. Introduction

Charge-ordering (CO) instability and associated anomalous behaviors of electrons have recently been one of the major topics in the field of strongly correlated electron systems. A well-known example is the vanadate bronze α'-NaV_2O_5 where the system may be modeled as a lattice of coupled ladders (or a trellis lattice) at quarter filling [1,2]. In this material, the CO with a zigzag ordering pattern is observed below $T_{CO} = 34$ K [3–5], and associated with this, a number of anomalous behaviors, which can be related to the slow dynamics of charge carriers (or charge fluctuation), have been observed above T_{CO} [4,6]. The spin degrees of freedom has also been reported to be anomalous [4,7]. We therefore want to consider how in such systems the spin degrees of freedom behave near the CO phase transition when they are on slowly fluctuating charge carriers.

One of the simplest models that allow for such situation is the anisotropic Hubbard ladders at quarter filling with the strong intersite Coulomb repulsion. We here use an effective Hamiltonian written in terms of the spin and pseudospin (representing charge degrees of freedom) operators [1,8–10], which may be written as a sum of the quantum Ising term for pseudospins and the spin-pseudospin coupling term:

$$H = J_1\Big(-\frac{g}{2}\sum_i T_i^x + \sum_i T_i^z T_{i+1}^z \Big) + J_2 \sum_i \Big(\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \frac{1}{4}\Big)\Big(T_i^+ T_{i+1}^- + \text{H.c.}\Big)$$

with the standard notation. $\mathbf{S}_i$ and $\mathbf{T}_i$ are, respectively, the spin and pseudospin operators of spin-1/2 at site i, where $T_i^z = -1/2$ $(+1/2)$ means the electron is on the left (right) site on the rung of the ladder. J_1 is the energy scale of the pseudospin system and J_2 is the coupling strength between the spin and pseudospin systems. We have so far used the quantum Monte Carlo (QMC) method to calculate the temperature dependence of the uniform spin susceptibility and the spin and charge excitation spectra, thereby clarifying consequences of the interplay between its spin and charge degrees of freedom [11].

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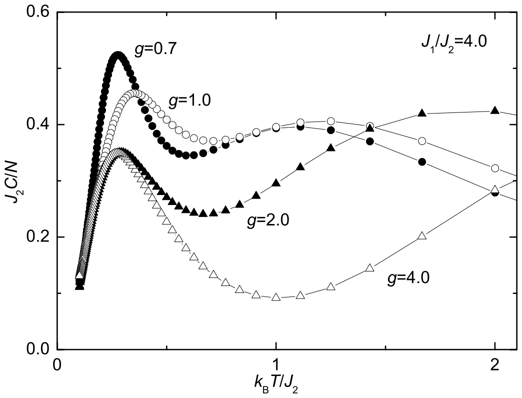

Fig. 1. Temperature dependence of the specific heat C calculated for our coupled spin-pseudospin Hamiltonian. The finite-temperature DMRG method [12,13] is used.

In this short article, we present the calculated results for the specific heat C of our model by the finite-temperature density-matrix renormalization group (DMRG) method [12,13] and show that the results reinforce our conclusion [11] that there is a parameter and temperature region where the spin degrees of freedom of our spin-pseudospin system are 'separated' from the charge degrees of freedom and their coupling leads to the anomalous spin excitations of the system.

2. Calculated results and discussion

We have shown [11] that, when the pseudospin quantum fluctuation is large ($g \gtrsim 1$), the dispersion relation of the spin exitation spectra of our model at low temperatures agrees well with that of the 1D antiferromagnetic Heisenberg model with the renormalized effective exchange coupling constant $J_{\rm eff} = 0.6J_2$ that is independent of the energy scale of the pseudospin system J_1. We have also shown that the temperature dependence of the uniform spin susceptibility of our model is well described again by the 1D antiferromagnetic Heisenberg model with the same effective exchange coupling constant $J_{\rm eff} = 0.6J_2$. The description is valid up to the crossover temperature T^* that is related to the pseudospin excitations of the system and roughly scales with J_2 unless the quantum fluctuation of the pseudospins is small ($g \lesssim 1$).

Now, in Fig. 1, we show that the temperature dependence of the specific heat of our model has a two-peak structure: a rather sharp peak appears at a low-temperature region $k_{\rm B}T \simeq 0.3J_2$ and a broad peak structure appears at a high-temperature region $k_{\rm B}T \gtrsim 0.8J_2$ when $J_1/J_2 = 4$. We find that the low-temperature peak can be fitted very well to the temperature dependence of the specific heat of the 1D antiferromagnetic Heisenberg model with the effective exchange coupling constant $J_{\rm eff} = 0.6J_2$; this value is in accord with the effective exchange constant estimated from both excitation spectra and uniform spin susceptibility. The temperature at which the deviation in the fitting occurs is at $k_{\rm b}T/J_2 \simeq 0.5 - 1$ depending on the value of g, which is also consistent with the estmate from the temperature dependence of the uniform spin susceptibility.

We note that the parameter values for α'-NaV_2O_5 may be estimated as $J_1 \sim 1.6$ eV, $J_2 \sim 0.10$ eV, and $g \sim 0.75$ [2]. Thus, this material may be in the region of $g \lesssim 1$, where the spin degrees of freedom are not completely separated from the charge degrees of freedom. The anomalous response of the spin degrees of freedom may therefore be expected as some experimental data [4,7] suggest; we hope that further experimental studies will be made to clarify this point.

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