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Nonquasiparticle states in the half-metallic ferromagnet simulated by the two-band Hubbard model

K Nakano[1], T Shirakawa[2] and Y Ohta[1]

[1]Department of Physics, Graduate School of Science, Chiba University, Japan
[2]Institut für Theoretische Physik, Leibnitz Universität Hannover, Germany

E-mail: ohta@science.s.chiba-u.ac.jp

Abstract. The density-matrix renormalization group method is used to study the three-band zigzag ladder model that simulates the electronic state of the t_{2g}-orbital system of the double string of the edge-shared CrO_6 octahedra in the half-metallic ferromagnet $K_2Cr_8O_{16}$. The saturated ferromagnetism caused by the double-exchange mechanism is thereby demonstrated. We also use the Lanczos exact-diagonalization technique on small clusters to study the two Hubbard chains coupled with the ferromagnetic exchange interaction, whereby we consider the nonquasiparticle states in the half-metallic ferromagnet that appear in the single-particle spectral function.

1. Introduction

Half-metallic ferromagnets [1] offer a unique opportunity for studying the electronic states of strongly correlated electron systems. Here, only the majority-spin electrons form the Fermi surface with a gapped minority-spin band and can couple with excitations of the spin (and in some cases orbital) degrees of freedom of the system. The situation therefore should attract much interest, in particular, when the relevant electrons are strongly correlated, leading the system to double-exchange ferromagnetism [2] and metal-insulator transition (MIT).

In this paper, motivated by a recent discovery [3, 4] that a chromium oxide $K_2Cr_8O_{16}$ with the hollandite-type crystal structure [5] belongs to this class of materials, we study electronic states of the three-band zigzag ladder model by the density-matrix renormalization group (DMRG) method. We also study the model of two Hubbard chains coupled with ferromagnetic exchange interaction by the Lanczos exact-diagonalization technique on small clusters. We thereby consider the origin of saturated ferromagnetism caused by the double-exchange mechanism and indications of nonquasiparticle states [1, 6, 7] appeared in the half-metallic ferromagnet within the simplest models.

2. Method of calculation

The crystal structure of $K_2Cr_8O_{16}$ belongs to a group of hollandite-type phases where one-dimensional (1D) double strings of edge-shared CrO_6 octahedra (see Fig. 1) forms a Cr_8O_{16} framework of a tunnel structure, wherein K ions reside [5]. Cr ions are in the mixed-valent state of Cr^{4+} (d^2) : Cr^{3+} (d^3) = 3 : 1, and hence with 2.25 electrons per Cr ion.

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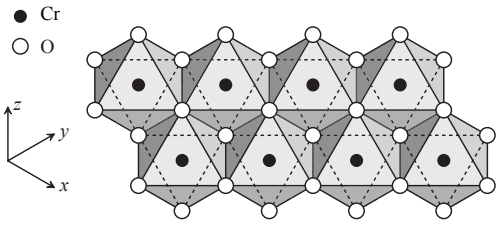

Figure 1. Schematic representations of the double string of the edge-shared CrO_6 octahedra in the hollandite structure.

To simulate the electronic states of this system, we use a model for the double string of Cr ions, retaining only the t_{2g} orbitals (see Fig. 2 for its schematic representation). Our Hamiltonian is therefore of the following form:

$$\begin{aligned}\mathcal{H} &= -\sum_{\langle i\alpha,j\beta\rangle,\sigma} t_{i\alpha,j\beta}(c^\dagger_{i\alpha\sigma}c_{j\beta\sigma} + \text{H.c.}) - J_{\text{H}}\sum_{i\sigma\sigma',\alpha\neq\beta} c^\dagger_{i\alpha\sigma}c^\dagger_{i\beta\sigma'}c_{i\beta\sigma}c_{i\alpha\sigma'} \\ &+ U\sum_{i\alpha} n_{i\alpha\uparrow}n_{i\alpha\downarrow} + U'\sum_{i,\alpha\neq\beta} n_{i\alpha}n_{i\beta} \end{aligned} \quad (1)$$

where $c^\dagger_{i\alpha\sigma}$ ($c_{i\alpha\sigma}$) is the creation (annihilation) operator of an electron at site i, orbital α, and spin $\sigma = \uparrow, \downarrow$. We define the number operators $n_{i\alpha\sigma} = c^\dagger_{i\alpha\sigma}c_{i\alpha\sigma}$, $n_{i\alpha} = n_{i\alpha\uparrow} + n_{i\alpha\downarrow}$, and $n_i = \sum_\alpha n_{i\alpha}$. J_{H} is the Hund's rule coupling, and U and U' are the intra- and inter-orbital on-site Coulomb repulsions, respectively. We assume the relation $U' = U - 2J_{\text{H}}$ throughout the paper, which is valid in the atomic limit. $t_{i\alpha,j\beta}$ is the hopping parameter between the orbital α on site i and orbital β on site j where $\alpha, \beta \in \{d_{xy}, d_{yz}, d_{zx}\}$ in the coordinate system shown in Fig. 1. We retain only the direct electron hopping between the t_{2g} orbitals for simplicity. We then have the independent nearest-neighbor hopping parameters t_a, t_b, and t_c as shown in Fig. 2.

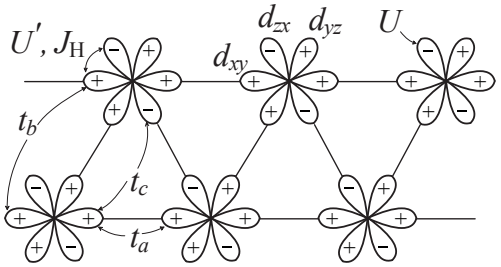

Figure 2. Schematic representation of the t_{2g} orbitals on the 1D zigzag chain of $K_2Cr_8O_{16}$. Two of the four lobes for each of the three t_{2g} orbitals are drawn.

We also use the two-chain Hubbard model with the ferromagnetic exchange interaction between the chains [8]. We calculate the single-particle spectral function defined as

$$A(\mathbf{q},\omega) = A^-(\mathbf{q},-\omega) + A^+(\mathbf{q},\omega) \quad (2)$$

with the electron removal spectrum

$$A^-(\mathbf{q},\omega) = -\frac{1}{\pi}\Im\langle\Psi_0|c^\dagger_{\mathbf{q}\sigma}\frac{1}{\omega + i\eta - (\mathcal{H} - E_0)}c_{\mathbf{q}\sigma}|\Psi_0\rangle \quad (3)$$

and electro addition spectrum

$$A^{+}(\mathbf{q},\omega) = -\frac{1}{\pi}\Im\langle\Psi_0|c_{\mathbf{q}\sigma}\frac{1}{\omega + i\eta - (\mathcal{H} - E_0)}c^{\dagger}_{\mathbf{q}\sigma}|\Psi_0\rangle, \tag{4}$$

where $\eta \to +0$, which is replaced by a small positive number in the actual calculations to give an artificial broadening of the spectra. We use a cluster of 16 sites with open boundary condition for these calculations.

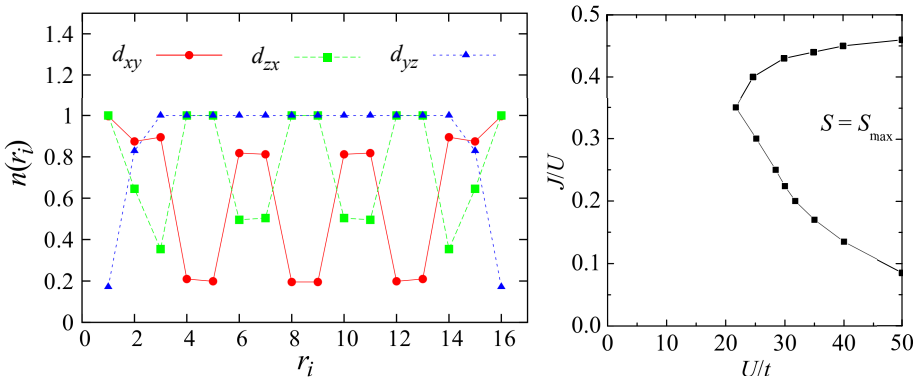

Figure 3. Left panel: Ground-state charge distribution of the three-band model calculated by the DMRG method. The result for the finite-size cluster of 16 sites (or 48 orbitals) with open boundary condition is shown, where we assume the values of the parameters $t_a = 1$, $t_b = t_c = 0$, $U = 30$, $U' = 10$ and $J_{\rm H} = 10$. Right panel: Ground-state phase diagram in the parameter space where we assume $t_a = 1$ and $t_b = t_c = 0$ with the assumption $U = U' + 2J_{\rm H}$. In both calculations, the cluster contains 36 electrons.

3. Results of calculation

Calculated results for the ground state of the three-band model are shown in Fig. 3. In the phase diagram, we find the fully spin-polarized region $S = S_{\rm max}$ for the large values of U. In this ferromagnetic region, we find that the electron distribution is characteristic of the fully occupied d_{yz} orbitals coexisting with the partially occupied d_{xy} and d_{zx} orbitals. Thus, we have a dualistic situation where the localized d_{yz} electrons interact with the itinerant d_{xy} and d_{zx} electrons via the Hund's rule coupling, resulting in the ferromagnetic spin polarization via the double-exchange mechanism [2]. One should note that the role of orbitals is different from that obtained in the generalized gradient approximation within the density functional theory where the d_{xy} electrons are essentially localized and the d_{yz} and d_{zx} electrons are highly itinerant [4]. The difference may come from the coupling between the double strings that is not taken into account in our simple 1D model calculations.

We also calculate the ground state of the two-chain Hubbard ladder model coupled by the Heisenberg-type ferromagnetic exchange interaction. We find the fully spin-polarized ground state in a parameter space (see Ref. [8]). In this parameter region, we calculate the single-particle spectral function. The result is shown in Fig. 4. We find that the metal-like spectra appear in the majority-spin spectral function (where a gap-like feature due to finite-size effect is expected to vanish in the thermodynamic limit), whereas the gap opens clearly in the minority-spin spectral function, indicating the system to be half-metallic. The indication of the presence of nonquasiparticle state is not clear although the state just above the Fermi level in the minority-spin spectral function may correspond to the state. Further studies are in progress.

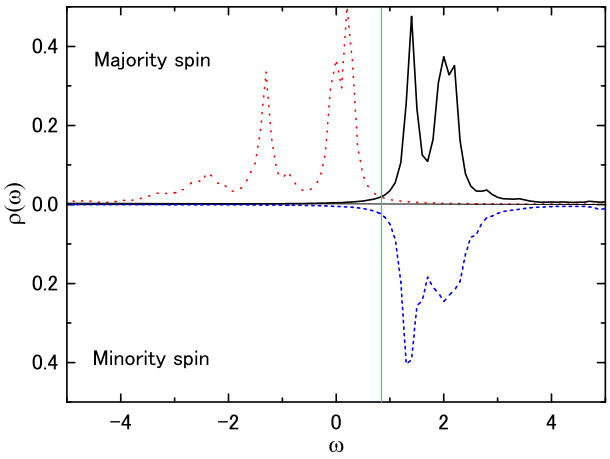

Figure 4. Momentum-integrated single-particle spectral function $\rho(\omega) = \sum_{\mathbf{q}} A(\mathbf{q}, \omega)$ calculated for the two-chain Hubbard ladder model. The vertical line indicates the Fermi level. We use a 16-site cluster with 6 electrons with the parameter values $t = 1$, $U = 30$, $U' = 10$, and $J = 10$, where the ground-state is fully spin-polarized.

4. Summary

We have applied the DMRG method to the three-band zigzag ladder model of the t_{2g}-orbital system and have studied the saturated ferromagnetism caused by the double-exchange mechanism, whereby we have simulated the electronic states of the half-metallic ferromagnet $K_2Cr_8O_{16}$ recently found. We have shown that the fully spin-polarized region actually appears in the ground-state phase diagram, where the fully occupied d_{yz} orbital coexists with partially occupied d_{xy} and d_{zx} orbitals, as is expected in the double-exchange ferromagnet. We have also studied the nonquasiparticle states in the single-particle spectral function by means of the Lanczos exact-diagonalization technique on small clusters of the two-chain Hubbard model. We have thereby discussed possible indications of the nonquasiparticle states appeared in the half-metallic ferromagnet, of which further studies are in progress.

Acknowledgments

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