Electronic states and metal-insulator transition in the triangular lattice *d-p* model for layered cobaltates

Yoshiaki ŌNO [a,b]

[a] *Department of Physics, Niigata University, Ikarashi, Niigata 950-2181, Japan*
[b] *Center for Transdisciplinary Research, Niigata University, Ikarashi, Niigata 950-2181, Japan*

Abstract

We investigate the electronic state of the 11 band *d-p* model on the two-dimensional triangular lattice simulating a CoO_2 plane in the layered cobalt oxides such as Na_xCoO_2 and $Na_xCoO_2 \cdot yH_2O$. The tight-binding parameters are determined so as to fit the LDA band structure. Using the slave boson approach together with the $1/N$ expansion method, we obtain the renormalized quasiparticle bands, where the a_{1g} band with a large hole Fermi surface is largely renormalized due to the strong correlation effect, while the e'_g bands with 6 hole pockets are almost unchanged. We also discuss the metal-insulator transition (MIT) with varying the *d-p* charge transfer energy Δ, and find that the MIT takes place at a critical value $\Delta_c = 4.01$ eV.

Key words: Na_xCoO_2, Triangular lattice, *d-p* model, Metal-insulator transition, Slave boson, $1/N$ expansion
PACS:

To investigate the electronic states of the CoO_2 plane in the layered cobalt oxides such as Na_xCoO_2 and recently discovered superconductor $Na_xCoO_2 \cdot yH_2O$ [1], we employ the two-dimensional triangular lattice *d-p* model with 11 orbitals: t_{2g} orbitals (d_{xy}, d_{yz}, d_{zx}) and e_g orbitals ($d_{x^2-y^2}$, $d_{3z^2-r^2}$) of a Co atom and 6 *p*-orbitals of two O atoms on the upper and lower sides of a CoO_2 plane. The noninteracting part of the Hamiltonian is given by

$$H = \epsilon_p \sum_{i\mu\sigma} p^+_{i\mu\sigma} p_{i\mu\sigma} + \sum_{imm'\sigma} \epsilon_d^{mm'} d^+_{im\sigma} d_{im'\sigma} + \sum_{ij\mu\mu'\sigma} t^{pp}_{ij\mu\mu'} p^+_{i\mu\sigma} p_{j\mu'\sigma} + \sum_{ijm\sigma} t^{dd}_{ijm} d^+_{im\sigma} d_{jm'\sigma} + \sum_{ij\mu m\sigma} (t^{pd}_{ij\mu m} p^+_{i\mu\sigma} d_{jm\sigma} + h.c.), \quad (1)$$

where $p^+_{i\mu\sigma}$ and $d^+_{im\sigma}$ are the creation operators for the p and the d electrons with site i, orbital μ (m) and spin σ, respectively. In eq.(1), the atomic energy for the d electron is explicitly given by: $\epsilon_d^{mm'} = \epsilon_d \delta_{mm'} + \frac{\Delta_t}{3}(1 - \delta_{mm'})$ for $m \in t_{2g}$, and $\epsilon_d^{mm'} = (\epsilon_d + 10Dq)\delta_{mm'}$ for $m \in e_g$, where Δ_t and $10Dq$ are the trigonal and the tetrahedral crystal electric fields, respectively. The *d-p* charge transfer energy is defined as $\Delta \equiv \epsilon_p - \epsilon_d$. The atomic energies together with the transfer integrals $t^{pp}_{ij\mu\mu'}$, t^{dd}_{ijm} and $t^{pd}_{ij\mu m}$, which are written by the Slater-Koster parameters, are determined so as to fit the tight-binding energy bands to the LDA bands for $Na_{0.5}CoO_2$ [2].

The ground state of the cobalt ion in Na_xCoO_2 is known to be a low spin state: $Co^{4+}(S = \frac{1}{2}, t^5_{2g}e^0_g)$ for $x = 0$ and $Co^{3+}(S = 0, t^6_{2g}e^0_g)$ for $x = 1$. Then, we assume the occupied states t^n_{2g} with $n \leq 4$ are excluded; which is reproduced by taking into account of the infinite Coulomb repulsion U between t_{2g} holes. The model can be described by the Hamiltonian eq.(1) with replacing $d^+_{im\sigma} \to f^+_{im\sigma} b_i$ for $m \in t_{2g}$, under the local constraints: $\sum_{m\sigma} f^+_{im\sigma} f_{im\sigma} + b^+_i b_i = 1$ for all i, where b^+_i is the creation operator for the slave boson representing the hole empty state

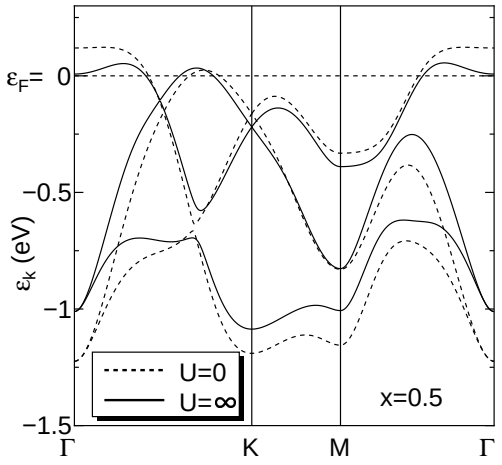

Fig. 1. The energies for the tight-binding bands (dashed lines) and those for the renormalized quasiparticle bands (solid lines) at $x = 0.5$ of Na_xCoO_2.

t_{2g}^6 and $f_{im\sigma}^+$ is that for the pseudo fermion representing the single hole state t_{2g}^5. As the e_g orbitals are almost empty due to a large value of $10Dq \sim 1.14$eV, the Coulomb interaction for e_g electrons together with that for p electrons is neglected.

Within the leading order w.r.t. $1/N$, where N is the spin-orbital degeneracy of t_{2g} and $N = \sum_{m\sigma} = 6$ in the present case, the Dyson equations for the single particle Green's functions are obtained and solved analytically at $T = 0$ as previously done for the periodic Anderson model [3] and the d-p model [4]. Then, the energies for the renormalized quasiparticle bands $E_{ks\sigma}$ are obtained by diagonalizing the renormalized Hamiltonian, $\tilde{H} = \sum_{s=1}^{11}\sum_{k\sigma} E_{ks} c_{ks\sigma}^+ c_{ks\sigma}$, which is given by eq.(1) with replacing $t_{ijm}^{dd} \to Z t_{ijm}^{dd}$, $t_{ij\mu m}^{pd} \to \sqrt{Z} t_{ij\mu m}^{pd}$ and $\epsilon_d \to E_d$. The renormalization factor Z and the renormalized atomic energy E_d are obtained by solving the following self-consistent equations:

$$1 - Z = \sum_{ksm\sigma} |v_{ksm}|^2 f(E_{ks}), \tag{2}$$

$$\epsilon_d - E_d = \frac{1}{2}\sum_{ks\mu m\sigma}\left(\frac{t_{k\mu m}^{pd}}{\sqrt{Z}} u_{ks\mu} v_{ksm}^* + c.c.\right) f(E_{ks}) + \sum_{ksm\sigma} t_{km}^{dd} |v_{ksm}|^2 f(E_{ks}), \tag{3}$$

where $u_{ks\mu}$ and v_{ksm} are coefficients for the unitary transformation diagonalizing $\tilde{H}$: $c_{ks\sigma} = \sum_\mu u_{ks\mu} p_{k\mu\sigma} + \sum_m v_{ksm} d_{km\sigma}$.

Figure 1 shows the energies for the renormalized quasiparticle bands together with those for the noninteracting tight binding bands at $x = 0.5$ of Na_xCoO_2, where t_{2g} bands with $s = 7, 8, 9$ are shown in the figure, while p bands with $s = 1 - 6$ and the e_g bands with $s = 10, 11$ are not shown. Due to the strong correlation effect, the a_{1g} band with a large hole Fermi surface around the Γ point is largely renormalized near the Fermi level, while the e_g' bands with 6 hole pockets near the K point are almost unchanged.

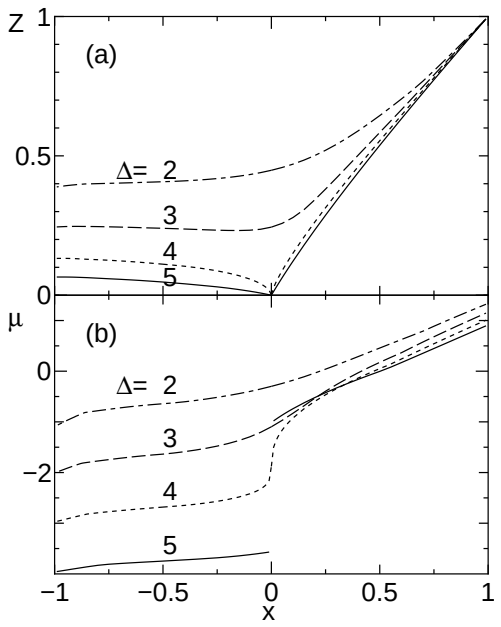

Fig. 2. The renormalization factor Z (a) and the chemical potential μ (b) as functions of x for several values of the d-p charge transfer energy Δ.

In Fig. 2, the renormalization factor Z and the chemical potential μ are plotted as functions of x, where the number of holes in the t_{2g} bands is given by $n_{\rm hole} = 1 - x$. When Δ is varied, the MIT takes place at a critical value $\Delta_c = 4.01$ eV: for $\Delta > \Delta_c$ the system is insulator at $x = 0$, while for $\Delta < \Delta_c$ the system is metallic even at $x = 0$. The critical value is larger than the LDA value $\Delta_{\rm LDA} = 1.8$ eV [2] and is comparable to the experimental value from PES $\Delta_{\rm PES} = 4$ eV [5].

This work was supported by the Grant-in-Aid for Scientific Research from the Ministry of Education, Culture, Sports, Science and Technology.

References

[1] K. Takada *et al.*, Nature **422** (2003) 53.

[2] D. Singh, Phys. Rev. B **61** (2000) 13397.

[3] Y. Ōno *et al.*, Physica C **159** (1989) 878.

[4] H. Jichu *et al.*, J. Phys. Soc. Jpn. **58** (1989) 4280.

[5] A. Chainani *et al.*, Phys. Rev. B **69** (2004) 180508.