Abstract Submitted for the MAR05 Meeting of The American Physical Society

Ferromagnetic spin fluctuation and possible triplet superconductivity due to inter-orbital Hund's-rule coupling in $Na_x CoO_2 \cdot yH_2O$ MASAHITO MOCHIZUKI, YOUICHI YANASE, MASAO OGATA, Dept. of Physics, Univ. of Tokyo — Electronic structure and superconductivity in $Na_x CoO_2$. yH_2O are studied theoretically by using a fluctuation- exchange approximation. This material has partially-filled Co t_{2q} orbitals and LDA calculation shows that its Fermi surface consists of more than two bands. Thus, we expect that the multi-band or multi-orbital contributes to the low- energy electronic state in this material. We employ a multi-orbital Hubbard model which includes the Co t_{2g} orbitals. Tightbinding parameters are determined to reproduce the LDA band dispersions. To analyse this model, we extend the fluctuation-exchange approximation to a triplydegenerate orbital case. We will discuss that several important and interesting aspects appear which are not expected in a single-band model. One of them is a ferromagnetic (FM) spin fluctuation which is enhanced by the inter-orbital Hund'srule coupling. This FM spin fluctuation leads to triplet pairing mainly on the disconnected hole-pocket Fermi surfaces, in contrast to the naive expectation of RVB superconductivity in a single-band t-J model. We will also discuss the obtained results in the light of available experimental findings. On the basis of these analyses, we will point out that $Na_{0.35}CoO_2 \cdot 1.3H_2O$ can provide a key material for clarification of roles of orbitals on the superconductivity in the strongly correlated electron systems.

> Masahito Mochizuki Dept. of Physics, Univ. of Tokyo

Date submitted: 30 Nov 2004

Electronic form version 1.4